Quantification of uncertainty and spatial variability of characterisation factors in the new global LCIA method IMPACT World+

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Use of antibiotics as growth promoting agents in livestock production contributes to the increasingly worrisome development of antibiotic resistance. In order to evaluate the long term impacts of antibiotic exposure on soil microbial populations, a series of field plots were established in London, Ontario, Canada in 1999 that have since received annual applications of a mixture of sulfamethazine, tylosin and chlortetracycline at concentrations (0, 0.1, 1.0 and 10 mg/kg soil) bracketing that which would result from an annual application of manure from medicated swine. Following ten annual applications, biodegradation potential and persistence of these drugs was evaluated. Residues of sulfamethazine and tylosin, but not chlortetracycline, were removed much more rapidly in soil with a history of exposure to the drugs than in untreated control soil. Residues of ^{14}C-sulfamethazine were rapidly and thoroughly mineralized to $^{14}CO_2$ in the historically treated soils, but not at all in the untreated soil. Enrichment cultures of bacteria able to degrade sulfamethazine were obtained from historically treated soils, but not from untreated soil. The abundance of viable bacteria and their relative distribution in major bacterial phylogenetic groups of bacteria was evaluated microscopically. Using DAPI and the Molecular Probes Live/Dead stain, there was no treatment effect on the abundance of viable bacteria. There were no differences between treatments with respect to the relative abundance of Alpha-*Proteobacteria*, Beta-*Proteobacteria*, Gamma-*Proteobacteria*, low-GC and high-GC Gram positive bacteria. There were differences in the abundance of Planctomycetes and the *Cytophaga-Flavobacterium* cluster with treatment, but these did not indicate a coherent dose-response. Long-term treatment altered functional microbial populations as detected using the pollution induced community tolerance (PICT) test evaluated with either each of the antibiotics present individually, or as a mixture. Overall, these results indicate that soil bacteria adapt functionally to long-term exposure to some veterinary antibiotics, notably resulting in sharply reduced persistence of the drugs. Accelerated biodegradation of antibiotics in matrices exposed to agricultural, wastewater, or pharmaceutical manufacturing effluents would attenuate environmental exposure to antibiotics, and merits investigation in the context of assessing potential risks of antibiotic resistance development in the environment.

ET19A-6
Effects of pig slurry co-applied sulfadiazine (SDZ) on the microbial diversity in soil microcompartments such as earthworm channels and rhizosphere soil
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Effects of veterinary antibiotics such as sulfadiazine (SDZ) on soil microbial diversity were previously reported to depend on the presence of easily available nutrient sources (e.g. pig manure) and the spatial proximity of agents and microorganisms. Antibiotic effects in rhizosphere soil and earthworm channels, however, are not well investigated. Hence, we determined antibiotic effects in two independent experiments using agricultural topsoil (Luvisol) mixed with SDZ spiked pig manure. Rhizosphere soils of maize plants were studied using the chloroform fumigation extraction (CFE) and phospholipid fatty acid (PLFA) analysis. In contrast to un-rooted bulk soil, microbial biomass and PLFA profiles substantially changed after applying more than 1ppm SDZ. Sections of Lumbricus terrestris L. channels were sampled after top application of SDZ spiked slurry and investigated using 16S rRNA gene denaturing gradient gel electrophoresis (DGGE) and enzyme activity measurements. The organic matter composition and wettability of earthworm channels were mapped by 2D-DRIFT-FTIR along transects. The experiment confirmed evident pseudomonas and ß-proteobacteria community shifts as well as a decreased C/N ratio at the inner surface of earthworm channels. The DRIFT mapping confirmed the larger hydrophobicity of inner earthworm channel surfaces, whereas the boundary layer to the bulk soil was more hydrophilic. These results show that the fate and effect of veterinary medicine has to consider the heterogeneity of natural soil environments.

ET19B-1
Effect of repeated application of sulfadiazine-contaminated pig manure on abundance, Diversity and activity of microbes involved in nitrogen transformation in different soil compartments
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Several studies from our group have indicated pronounced effects of single application of sulfonamide (SDZ) contaminated manure to soil. The aim of this study was to investigate the effects of the antibiotic sulfadiazine in combination with pig manure on the abundance, diversity and activity of functional microbial communities involved in nitrogen (N) transformation in different soil compartments after repeated application of the antibiotic. The repeated applications of SDZ-contaminated manure to bulk soil entailed different response patterns of functional genes involved in N cycling after the first, the second and the third amendment which might indicate an adaptation of the microbial communities to the antibiotic substance.

ET19B-2
The effect of sulfadiazine on bacterial dynamics in the field
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A kinetic model that couples environmental fate processes of antibiotics with an effect model of bacteria inhibition was studied. The model uses the antibiotics concentration in soil as link. It requires a number of input parameters which are more or less uncertain. A probabilistic Monte-Carlo type methodology was used to estimate the uncertainty of selected output variables depending on uncertainty estimates of input parameters. Additionally, the contribution of single parameters to the simulated variability of the output is analyzed and expressed by the contribution to variance. The uncertainty of the output variables is characterized by the 10th and 90th percentile of the frequency distributions. As an example, sulfadiazine (SDZ) effect on the densitiy of ammonium-oxidizing bacteria (AOB) in soil was investigated. After manure application to soil, simulated SDZ concentration decreases monotonically with moderate uncertainty in the first 25 days. The time point at which the available SDZ concentration falls below the inhibition constant of AOB (0.025 mg/kg) is predicted to be most likely between 22 days (10th percentile) and 33 days (90th percentile). Increasing AOB densities over the first 15 to 50 days are predicted due to enhanced growth after amendment of ammonium containing manure. Once all ammonium has been consumed, AOB density decreases again. Uncertainty of the input parameters manifests itself in a difference of approximately factor 1.6 between the 10th and 90th percentile of AOB densities. A delaying effect of SDZ on AOB growth is predicted by the coupled model. Since in the first 22 - 33 days available SDZ is above the inhibition constant, growth of AOB is suppressed, but starts after SDZ has dissipated. The uncertainty is larger in the coupled model because it additionally carries the uncertainty of the chemical fate parameters. The contribution of the chemical fate parameters on AOB uncertainty is small compared to the parameters of the biological model. Only the hydrolization rate constant contributes to more than 20%. The analysis shows that the combined parameter uncertainty does not compromise the conclusion of the delaying effect of SDZ on AOB growth after manure amendment. The probabilistic simulations show that the chemical fate model, the AOB growth model and the coupled model deliver interpretable predictions of the dynamics of the important output variables SDZ and AOB, even with the uncertainty of the input parameters.

ET19B-3
Modelling environmental risks of veterinary medicines used in Asian pond aquaculture
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A wide array of Veterinary Medicinal Products (VMPs) have been introduced during the last decades in Asian aquaculture production for treating and preventing bacterial diseases and parasitic infestations in the cultured species. In the present study, a decision support system (ERA-AQUA) was developed to assess risks of VMPs applied in Asian pond aquaculture for the targeted produce, for human health and trade, and for surrounding aquatic ecosystems. VMP concentration dynamics are modelled in four different compartments (i.e., pond water, pond sediment, cultured species, and the watercourse receiving effluent discharges) based on scenario and physico-chemical input parameters, and mass balance equations. Predicted no effect concentrations (PNECs) for the targeted produce and acute and chronic PNECs for aquatic organisms (i.e., algae, invertebrates and fish) are calculated from toxicity data and assessment factors according to international risk assessment guidelines for VMPs. Acceptable daily intakes and maximum residue levels are used to assess risks for consumers and trade, respectively. Finally, risk quotients are calculated for each of the included endpoints and the potential exceedance of the predicted exposure concentrations over the calculated "safe"concentration is provided by the model. In this presentation, the model will be presented and its potential applications will be demonstrated through a case study in which risks will be assessed for the application of oxytetracycline (antibiotic) and benzalkonium chloride (disinfectant) in an intensive striped catfish (Pangasianodon hypophthalmus) scenario for the Mekong Delta (Vietnam). The ERA-AQUA decision support system can be considered as a useful tool i) for performing preliminary risk assessments of VMPs applied in Asian pond aquaculture, ii) for assessing the influence of different application schemes and aquaculture practices on the environmental impacts of aquaculture production, and iii) for designing chemical and biological monitoring and other higher-tier risk assessment studies.

ET19B-4
Effects of ivermectin application to cattle on dung fauna and dung degradation: an international comparison of field studies
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It has been well documented that the application of toxic anthelmintics such as ivermectin to domestic animals can affect populations of dung-dwelling organisms and in some cases retard dung degradation. During the registration process, parasiticides such as anthelmintics need to be tested at higher tier levels (i.e., multi-species) when adverse effects on dung organisms are observed in single species toxicity tests. An outline for conducting such field tests was recently published. Following publication, an international project was set up in order (1) to assess the robustness of these field tests when conducted by different research groups at different geographic sites, varying in dung and soil faunas, and in environmental conditions, and (2) to investigate the effects of these variable conditions on the interpretation of test results. The experiments were conducted in Lethbridge, Alberta, Canada, near Montpellier, France, near Zurich, Switzerland, and in Wageningen, The Netherlands. Ivermectin was used as the test compound. The study demonstrated that there are considerable differences in the composition of the principal groups of dung insect fauna (family level) between different experimental sites in the study, as could be expected according to biogeography. The results further indicate that ivermectin does negatively affect various groups of dung flies and also dung beetles at the different study sites. However, ivermectin treatments do not seem to have an effect on the degradation rate of cattle dung in temperate climate regions. The study design is suitable to evaluate the effects of parasiticides on dung insects under field conditions such as required in higher-tier testing for risk assessment. Extreme weather conditions during the course of the experiments, however, may interfere with the abundance of certain important groups of dung insects.

ET19B-5

In vitro effects of 17β trenbolone on the mRNA levels of steroid hormone receptors, Growth Hormone and gonadotropins in pituitary glands from rainbow trout (Oncorhynchus mykiss)

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Based on the high biological activity of trenbolone in fish and on the doses used by body builders, the compound might potentially pose a risk to the aquatic environment also in EU although not officially present. Previous studies in our laboratories have shown that trenbolone is capable of irreversibly changing sex ratios to 100% males in zebrafish at water concentrations in the low ng/L level. The present study was undertaken to investigate effects of trenbolone on mRNA levels of steroid hormone receptors, GH, LH and FSH in pituitary glands from rainbow trout after in vitro incubations of the excised tissues with the synthetic androgen.
IGF-1 and AR mRNA levels in liver slices incubated with trenbolone at concentrations from 5-100 ng/ml were unchanged
Pituitary glands were incubated with trenbolone from 1.35-1355 pg/ml:
- No significant changes were found in GH mRNA levels
- AR mRNA was significantly reduced at all concentrations
- FSH mRNA was significantly incresed at the highest concentration
- LH mRNA was massively and inversely reduced with incubation concentrations

LC01 - Development in life cycle inventory analysis and modelling

LC01A-1

Market-based allocation of recycling benefits

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Market-based allocation of recycling benefits has already been described since the years 2000. However, this approach tends not to be largely adopted in international standards.
In practice, there are mainly three types of benefit allocation with system expansion modeling: (i) allocation of benefits to the producer bringing material on the market (that can become secondary material at end-of-life); (ii) allocation to the product incorporating secondary material and (iii) 50/50 allocation (half of the benefits of recycling at end-of-life and half of the benefits of incorporating secondary material are accounted for).
Market-based allocation is dictated by the answers to the following questions: "Which additional amount of secondary material will be exchanged on the market if supply increases thanks to the apparition of a new source of secondary material?" or "Which additional amount of secondary material will exchanged on the market if demand increases thanks to the apparition of a new producer of a good based on the secondary material?" Analysis of price elasticity of demand and supply provides answers.
This paper aims at depicting several typical supply-demand curves and at associating these to actual market situations (for example, what if there is a back obligation or subsidized waste collection, etc.). The appropriate market-based allocation can hence be dictated in each case.
Namely, allocation to the supplier (i) is to be promoted in cases where the supply is fully inelastic and where the demand is fully elastic. Examples of such markets are, among others, PET and packaging glass.
In markets where answers to supply and demand variations are more equilibrated, a 50/50 allocation should be used, as it is the case for certain types of paper and boards.
Market situations for main materials are analyzed so as to provide sound justification for standard developments.

LC01A-2

Using a long-term energy model for the consequential and prospective life cycle assessment of the use of biomass based synthetic diesel (BTL) in France

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Consequential Life Cycle Assessment (C-LCA) has been developed recently as a modeling approach that captures environmental impacts of a product beyond direct physical relationships accounted for in Attributional LCA. This approach seems interesting for the evaluation of biofuels since their indirect impacts on other sectors (agriculture, forestry, electricity production) may be important. In this study, we use a prospective optimization model representing the French energy production and transportation sectors (agriculture is partially included due to the presence of biofuels) to evaluate the impacts of the production of BTL in France in the time horizon 2007-2030. The model was developed with the economic model generator TIMES.
Part of the work consisted in adapting the model to perform C-LCA integrating energy consumptions and emissions factors to the technologies described in the model. Scenarios were built in order to expose the C-LCA methodological issues we aim to discuss. We observed how the model behaves when applying variations to: the technology used for BTL production, the levels of development of BTL in France and the energy policy. Global Warming Potential (GWP) was calculated for each scenario using time-dependent characterization factors for greenhouse gases.
Preliminary results show that the long-term energy model can be applied for measuring the indirect effects of the development of BTL in France. For example, it was possible to identify the source of the electricity that is going to compensate the supplementary demand for electricity due to the production of BTL using an allothermic process. This type of model presents some advantages in relation to other models previously used in C-LCA:
- It allows a fine description of transformation steps of primary resources in energy carriers.
- It allows the observation of marginal and non-marginal perturbations on the energy sector.
- Emissions are endogenous to the model. Most of the other C-LCA studies use economic equilibrium models to quantify the consumption of certain products and the emissions are integrated manually afterwards.

Nevertheless, in this version of the model, the agricultural sector is only described partially and land use changes (direct and indirect) can't be evaluated. A whole world description of the agriculture and forestry sector would be necessary for this type of analysis. One way of improving this C-LCA would be to integrate our model with a general equilibrium model.

LC01A-3

Modelling land use changes in consequential LCI: limitations of equilibrium models

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This presentation aims at discussing the use and limitations of economic equilibrium models for the development of consequential LCI, with a specific focus on the case of biomethane production from maize in Luxembourg. The core research objective is the development and application of a Partial Equilibrium (PE) model representing the market constraints and reaction to the demanded production of maize and providing: 1) the change of crop production patterns, i.e. the primary consequences on Luxembourg's agriculture system. Forage crops are included, making the link to the consequences on meat and milk production. 2) The changes of land use type and related primary consequences in terms of modified pollutant emissions and land transformation impacts. The modelled changes are then propagated inside the national economy, using a computable general equilibrium model (Luxgem), and outside the national boundaries to account for additional environmental impacts.
So far the results show no need for intensification of the existing and new areas to meet demand for maize. To study the impacts of increased agriculture prices, we increased the import prices of the "agriculture" commodity by 10% in Luxgem calibrated to the base year 2005. We find that the share of expenditure by households on agriculture products fell from 2.5% to 2%. Agriculture has a very small share in the value added in the economy and increased demand for maize which may displace existing crops will not have serious economic impacts. These findings were corroborated using the global model GTAP, which was used to evaluate the increased demand for displaced agriculture crops on account of additional production of maize. However, since the PE model is based on revenue maximization, it is difficult to properly consider non-economic constraints such as behaviours related to habits, cultural heritages or additional regulatory constraints. Also the modelling of the influences of crop production patters on the food sectors is not trivial because of the difficulty of assigning a clear and robust aggregated market relation between forage crops and meat and milk.

Equilibrium models fall short in including non technical and non economical constrains. The complementary use of agent-based modelling could be an alternative approach for proper consequential LCI.

LC01A-4

Integrating accident-related methods and impacts into the life cycle toolbox

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Life Cycle Assessment is more and more understood to be 'only' one component of a wider environmental and even sustainability assessment toolbox. Enhancing classical Life Cycle Inventory (LCI) modelling by integrating accidents in production, use and end-of-life of products is one important step towards more complete evaluation of product systems' life cycles. LCA according to ISO 14040ff deals implicitly with non-accidental ('regular') releases only, while some accidental releases may be included due to how LCI data is collected (e.g. site's yearly average, including leakages etc.). There are however important organisational and decision-making related reasons for managing these two sets of inventories separately. Accident prevention in industry is done separately from dealing with normal releases to the environment. A separate inventory of accident related releases and casualties (Life Cycle Accident Inventory, LCAI) is hence required for effective decision support. Several studies present case-specific solutions for this issue and some general method concepts have been presented. A systematic and consistent methodological solution for full implementation is still lacking. Joining LCI methodology and tools from Risk Assessment (Event Tree Analysis and Fault Tree Analysis) yields a powerful approach for integrated analysis of the environmental and health effects from accidents and under regular operation. Moreover the methodological question comes up on how to reflect attributional and consequential modelling principles when modelling accident inventories for joint analysis with LCI data. The presentation will systematically address the question of how best to place the accident-related impacts within the life cycle toolbox and which methodological implications this has. Data sources and data management are further issues to discuss to ensure a proper approach in support of life cycle based decision making in industry.

LC01A-5

Better characterising the environmental performance of intermittent power generation with help of LCA: integrating wind power into the German electricity grid in 2006

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Intermittent power generation and in particular wind power is continuously gaining shares in the power plant parks of many countries. Given its intermittent nature, however, the true environmental impacts increased wind power integration remain an open question. This is because the seemingly equivalent functionality expressed in a kWh of electricity produced is in fact not directly comparable to conventional power generation techniques. For that reason, a more systemic approach is advocated. Relying on energy systems analysis results, the purpose of the study is to analyse to what extent considering substitutional effects and back-up can help better characterise power generation from intermittent resources. The study starts with describing the German electricity grid in 2006 with and without wind power generation. By using the results from an agent-based energy system model, the issues of intermittency and the backup needed for wind power were addressed. Through substitution of fossil fired capacities, the LCA considering these consequences led to an even better environmental performance of wind power in all of the considered impact categories (including global warming) compared to the LCA not considering these consequences, except for mineral resource depletion and natural land transformation. As this study could not fully resolve the issue of finding a functional unit that is more appropriate than the kWh for comparing different power generation techniques, other approaches are also discussed.

LC01B-1

Book, trade and claim systems in LCA: how to model certificates delinked from physical flows

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In May 2011, the association of issueing bodies AIB announced that 1 billion EECS certificates (which equals 1 billion MWh of electricity) have been issued in Europe since its start nine years ago. There is a large demand in renewable energy certificates, which helps electric utilities and companies from the manufacturing as well as service sector to reduce the environmental impacts of the electricity they purchase.
The international standards on life cycle assessment (ISO 14040, ISO 14044) do not specify how certificates should be taken into account when performing a product or company life cycle assessment (LCA) study. The recently completed carbon footprint standard are clear with regard to carbon offsetting measures (emission certificates): these are considered as a improvement measure and shall not included in the product LCA but kept separate.
Up to now, the role of renewable energy certificates has not been discussed widely. This presentation shows the mechanism and volume of RECS certificates as well as its consequences and proposes some guiding principles how RECS certificates may or may not be used within product LCAs and the eco-balances of companies.
During the last years, countries with large shares of hydroelectric power exported significant amounts of RECS certificates to other European countries. These RECS certificates are used to lower the carbon footprint of electricity purchased by companies and electricity providers. Thus the exports are compensated by imports of the same amounts of non renewable electricity qualities. This leads to substantially higher carbon intensities of the electricity mix of exporting countries.
We therefore recommend to disregard independently traded RECS certificates in product and service LCA as long as the LCI of national electricity mixes is based on international statistics disregarding RECS trade. If RECS certificates are linked to the production and delivery of renewable electricity, we recommend to include the respective share of renewables in the electricity mix.

LC01B-2

Using water markets and consequential LCA to assess indirect impacts from water use

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Using water can incur direct impacts on human health from water deprivation for domestic use or agriculture. However, these impacts do not occur in regions where economic resources are sufficient to allow the deprived users to turn towards technology to meet their needs. On the other hand, this technology leads to burden shifting that should be captured in a comprehensive assessment of water use in LCA. This paper proposes a consequential framework and model using water markets and marginal technology in order to assess LCA indirect impacts from water consumption and degradation, by identifying marginal processes and including their life cycle inventory. Adaptation occurs when a given type of water withdrawn, defined by its source and quality, is constrained. The assessment whether a water type is constrained or not is performed through a scarcity parameter, with the underlying assumption that an unconstrained resource is not scarce. The market concept, applied to water, is then used for each water type to consider all sources for this water type. These include available water of this type, treated water from a lower quality source of water, desalinated water, and imported water. Additional processes are associated with each of these source of water.
Results consist of quality-specific marginal water source available for 808 hydro-economic cells worldwide, as defined in Boulay et al, resulting in 6464 (808 cells x 8 water types) marginal processes which can then serve as input to the inventory and be assessed by any impact assessment methodology. Preliminary results are plotted on a world map giving additional energy demand incurred by the marginal processes for a 1000 m3 of good quality surface water use for each 808 hydro-economic cells.
This paper presents a novel approach assessing indirect impacts from water use due to compensation scenarios. It is especially relevant for developed countries facing water scarcity and/or poor water quality by overcoming current methodological limitations that solely consider direct impacts on human health from water deprivation. This model is based on a consequential approach, identifying the unconstrained marginal water source and treatment processes required to compensate the deprivation from water use.

LC01B-3

Modelling of biogenic CO2 fluxes in LCA and their integration with the global C cycle

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In Life Cycle Assessment (LCA), the same characterization factors are conventionally applied irrespective of when the emissions occur (the same importance is given to emissions in the past, present and future). This accounting paradigm makes bioenergy systems climate neutral as long as they are carbon neutral (the same amount of CO2 released from combustion is sequestered by growing trees). When the analysis is constrained by specific time boundaries the validity of this convention becomes shaky.
We stress the fact that the equivalency between C and climate neutrality in bioenergy LCA ignores the temporal gap between the emission (usually at a single point in time) and the sequestration flux, which is usually distributed over many years. Negleting these dynamics has an influence on the final climate impact assessment. The challenge for LCA practitioners is to model these fluxes and calculate the resulting climate impacts with unit-based indicators that be included in LCA case studies.
In this work, we elaborate on this issue using relatively simple mathematical methods which provide simulations of the carbon flow dynamics of biomass systems. Probability distribution functions are used to include in LCA the dynamic profiles of CO2 emissions and removals associated with biomass management for bioenergy and wooden products. Following an approach based on Impulse Response Functions, CO2 atmospheric profiles are calculated together with the respective changes in radiative forcing. Results show the importance of using emission and removal functions rather than single pulses or linear amortization procedures, which generally overestimate the climate impact of CO2 emissions, especially in presence of short time horizons and for relatively wide time-distributed emissions.
This method is flexible and can provide outcomes that are suitable to be routinely applied in LCA. Following this, we believe that a debate should be open in the LCA community to properly address timing of emissions and revisit the climate metrics used in the assessment. Besides normalized metrics as GWP, absolute metrics showing how the impacts change over time are preferable and can provide additional insights on the effective mitigation potentials of the system under study. The approach presented here deserves future research for a possible use in accounting of emissions from harvested wood products and in processing data by emission inventory experts within the Kyoto protocol and its successor.

LC01B-4

Evaluating the greenhouse gas emissions of retrofitting the existing Irish housing stock - A combination of process analysis and input-output analysis

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Historically, in Ireland focus has been on the domestic greenhouse gas emissions to the neglect of the emissions attributable to imports in retrofitting the existing Irish housing stock. This paper reports on a life cycle study of energy efficient retrofit options for the existing Irish housing stock with a focus on the significance of greenhouse gas emissions due to imports in order to depict the true total emissions attributable to retrofitting the existing Irish housing stock. While typical commercial LCA software tool was used to assess environmental impacts due to imported goods, domestic generated emissions including those due to imported products induced by addition of energy inputs were evaluated using input-out analysis. Results show that imports caused about 50% of the total greenhouse gas emissions. Although operational phase consumption and emissions was much greater than any other phase, there was a wide variation in the impacts on this balance across the retrofit options. Using these results an appraisal is provided of the benefits of utilizing process-based hybrid LCA to provide greater information to aid policy making on the life cycle performance of existing dwellings.

LC01B-5

A framework for prospective hybrid life-cycle assessment and its application to energy technologies

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Life-cycle assessment and input-output analysis literature abounds with case studies that have been developed at a particular place and a particular time in the past, being as many photographic representations of specific systems. In this literature body, analyses addressing future situations in which products will be produced, utilized and disposed are rare. Some are based upon optimization and equilibrium models. With the remarkable exception of the NEEDS project, future life-cycle inventory or input-output databases are not available. There is nonetheless an ever-increasing need for a life-cycle capable scenario modelling framework. We propose here a procedure to adapt life-cycle assessment (LCA) databases and multi-regional economic input-output (MRIO) tables to future years (up to 2050) according to various external parameters that have been identified as central in determining the environmental impacts of the overall economy. The EXIOPOL project has recently produced a highly detailed input-output model; we utilize this model to build a life-cycle based framework for scenario modelling. A combination of existing prospective studies, including International Energy Agency's are used to produce a consistent hybrid model of the world economy which can serve as the background for prospective life-cycle assessment studies. We present the model development and provide some basic comparisons of the scenarios implemented. Finally, in order to exemplify the use of such a prospective hybrid LCA model, we apply it to the integrated environmental assessment of selected low-carbon electricity production technologies.

LC02 - Developments in life cycle sustainability assessment

LC02A-1

UNEP/SETAC approach for a life cycle sustainability assessment of products - just in time

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Context

Every day, unsustainable patterns of consumption and production methods as well as population growth challenge the resilience of the planet to support human activities. At the same time, inequalities between and within societies remain high - leaving billions with unmet basic human needs and a disproportionate vulnerability to global environmental change. To counteract this trend, UNEP and SETAC (Society of Environmental Toxicology and Chemistry) have worked together through the UNEP/SETAC Life Cycle Initiative (Initiative) to develop the current work Towards a Life Cycle Sustainability Assessment (LCSA) . A key objective of the Initiative is to help extend life cycle assessment (LCA) methods and practices. This approach towards a LCSA bases on ISO 14040/44, ISO 26000 and acknowledges the developments of number of international initiatives and experiences about sustainability assessment. This publication is a natural step in UNEP's work, which has in the past decade focused on developing the 10-Year Framework of Programmes for Sustainable Development and which is now also focusing on economic sustainability through the UNEP Green Economy Initiative.

Scope

This publication describes life cycle techniques that can measure sustainability and allow LCA to support decision-making toward more sustainable product and process systems. An (Environmental) LCA looks at potential impacts to the environment as a result of the extraction of resources, transportation, production, recycling and use and discarding of products; life cycle costing (LCC) is used to assess the cost implications of this life cycle; and social life cycle assessment (S-LCA) examines their social consequences. However, in order to get the 'whole picture', it is vital to extend current life cycle thinking to encompass all three pillars of sustainability: (i) environmental, (ii) economic and (iii) social. This publication shows how all three techniques - which all share similar methodological frameworks and aims - can be combined to make the move towards an overarching LCSA possible.

Conclusion

LCSA has significant potential to be used by enterprises, governments, agencies for international cooperation and other organizations in society (such as consumers' associations) in their efforts to produce and consume more sustainable Still more research and applications are needed, but its application is already feasible and encouraged to speed the learning curve of the society.

LC02A-2

Challenges in implementing Life Cycle Sustainability Assessment (LCSA) and in an LCSA-based decision-making

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Life Cycle Sustainability Assessment (LCSA) has been proposed to be a combination of three assessments: environmental, economic and social (incl. socio-economic). In this way LCSA tries to make a bridge between the traditional environmentally oriented and generic life cycle assessment (LCA) and the more site- and time-specific sustainability assessment (SA), which takes into account all three generally accepted pillars of sustainability (economic, social and environmental). In the process of trying to bridge and to draw from the strong characteristics of SA and LCA, LCSA encounters its own challenges.

LC02A-3

Sustainability and human labour: how can LCA answer?

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In LCA the intrinsic dependence of productions on human labour (HL) is usually disregarded, without providing any clear argument. Apparently, HL is not considered to be related to and affected by, changes to the functional unit. Nevertheless, HL could be seen as the common numeraire among the three pillars of sustainability: environment, economy and society. This research aims at investigating the relationship between HL and LCA and at developing an operational framework to include HL in LCA. We defined three HL types (qualified worker, technician, manual worker). A comparative LCIA of the HLs types was carried out using an environmentally extended input-output model of EU-27. Afterwards, ten agri-food and industrial LCAs case studies were modified for hybrid LCAs, adding HL inputs to existing LCIs. The LCIA comparison showed that a qualified worker always generates impacts greater than other workers. The impact of average HL is higher in EU countries with the highest household expenditures' budget. Within the case studies, the HL significantly contributes to the total impact for several categories (e.g. fossil and ozone depletion up to 16% and 20%, respectively). We argue that an eco-profile of HL should always be added to LCI models that entail a significant direct human contribution: adding inputs of HL to the LCI of a product or process can improve its accuracy. This could enable to establish a common framework (same LCI) to account for HL under the three pillars of the life cycle sustainability assessment. So far, additional cost and social/organizational data of HL might be integrated in LCIs to provide useful information and an added value for more comprehensive assessment of the real life cycle cost (e.g. through addition of salaries and wages to the Life Cycle Costing (LCC) analysis) or social quality factors of labour (e.g. through implementation of further labour impact categories in the Social Life Cycle Assessment - SLCA) in a production chain. The proposed methodology can be used for a future implementation of HL at a level of unit process in LCA. By using a hybrid approach, possible double counting with non-human (i.e. machine driven) labour is easily avoided. However, humans are not machineries and they are driven by flows of information, knowledge, educational and cultural experience, and so forth. These are essential items for our future sustainable development but how to integrate them into human labour LCI profiles remains an open task.

LC02A-4

What life cycle sustainability assessment does and does not for new and innovative technologies

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Performing a sustainability assessment of new and innovative technology is a complex task, as showed by the definition itself, which refers to two big issues: Technologies

and Sustainability. Technologies can be classified in many ways, depending on the different typologies, development levels, effects and impacts on sectors, territories, markets, etc. The relation with sustainability is twofold, because technology can be considered both a cause of many environmental problems and a key to solve them. In fact, technologies are today considered the main agent of the present industrial, economical and social evolution and the main cause of the high speed of the present changes. As far as sustainability and sustainable development are concerned, they are very controversial and disputed at scientific and social level. Indeed, the sustainable development cannot be considered simply a goal, rather a social process where shared sustainability principles are considered as starting point for assessing decisions through an interactive learning process.
Being sustainability a global concept, inevitably calls for a system-wide analysis, a perspective that is at the core of the life cycle approach. A framework for life cycle sustainability analysis has been proposed, namely LCSA, which requires the application of LCA, Life Cycle Costing (LCC) and Social Life Cycle Assessment (S-LCA) under specific consistency requirements. The framework has been applied to the assessment of an innovative technology, in order to test its applicability, and it turned out to be a challenging task, mainly in relation to the following aspects: use of identical system boundaries; data availability and their significance; functional unit definition, especially in the case of S-LCA, and scenarios vs. product analysis. On the other side, the framework showed also its strenghts in forcing practitioners in thinking about the different options, and thus in detecting important aspects that at first sight could be considered negligible. However, we suggest supporting the application of the present LCSA with other methods and tools, able to take into account also aspects like the different ethical values, risk elements and the concept of social acceptance. Thus, LCSA can learn from the field of Technology Assessment in the way in which the problem is dealt with: the technology is at the core of the analysis, but the infrastructure and the organisation around it are equally important ingredients.

LC02A-5
Best Available System (BAS) for municipal solid waste management in developing Asian countries
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Fast growing mega cities in developing Asian countries are faced with municipal solid waste management (MSWM) related problems due to rapid urbanization, industrialization and population growth. Proper waste management with energy and material recovery prolongs the life of existing landfills, contributes in providing renewable energy and reduces pollution.
Although the need of shifting from landfilling to more environmentally sound solutions of solid waste management system is obvious, developing Asian countries have their own way of thinking, lifestyle, culture, budget related issues and concerns that reflects on their social and economy priorities in their decision making. For example, the fact that many scavengers lives depend on collecting and reselling plastic waste from the landfill to private recycling plants may interfere with the calorific value requirement of an incineration plant.
This study attempts to take into account the social and economy related considerations in Life Cycle Assessment (LCA) by using an integrated, survey based methodology called Environmental Load Point (ELP) developed in Nagata laboratory of Waseda University. ELP has broadened indicators categorized in 9 impact categories, which are energy depletion, global warming, ozone layer depletion, acid precipitation, resource consumption, air pollution, ocean and water pollution, waste disposal, and ecosystem influence. The ELP result is weighted with text mining factors from the national newspapers to find out the importance of each impact categories in the concerned country. Additionally, Life Cycle Cost (LCC) is combined with ELP results to give cost estimation of the constructed scenarios. This combination is called Best Available System (BAS) for MSWM. ELP represents the social considerations while LCC represents the economy factor of sustainability.
Different scenarios are constructed in this study with different portion of waste being recycled and incinerated, considering the composition of local waste and number of employment opportunity of scavenger in the new systems. BAS result may help decision makers to determine how far they should compensate with the lost of job market as well as taking a better MSWM technology with higher confidence because it has incorporated the ecology, economy, and social concerns. Moreover, text mining result is a reflection of the national concerns and priorities, thus it increases agreeability among the related community.

LC02A-6
Towards comparative life cycle sustainability assessment of road marking systems
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Public purchase decisions must cope with shrinking budgets at one hand and increasing demand for environmentally friendly products on the other. This study looks at both economic and environmental impacts of road markings considering the whole life cycle from manufacturing to disposal. For the first time all four major binder-based raw material options are evaluated that can be considered to equip a road section with road markings that provide high visibility even at wet nights for a period of ten years. For the accuracy of the study an external expert panel has reviewed the assessment.
Social aspects are considered in a second step. It is not trivial to quantify these.

LC02B-1
Evaluating multiple dimensions of sustainability in the case of bioenergy production based on multi-criteria analysis and life cycle assessment
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Environmental impacts of products and services have been traditionally the main focus in life cycle assessment (LCA). Recently, also other dimensions of sustainability including economic, social and even cultural aspects have been received more and more attention in addition to ecological impacts. Multi-criteria analysis (MCA) is a toolbox of methods that evaluate the properties of decision alternatives with respect to multiple, usually conflicting decision criteria.
First, this presentation discusses how MCA can be utilized in LCA when evaluating the sustainability of products and services. The most important benefits of MCA are connected to integration of impact assessments not measured directly in commensurable units and incorporation of subjective preferences into to the assessment framework. In general, the performance of decision alternatives depends on the weights given to various decision elements of the decision hierarchy and the performance of the decision alternatives with respect to the lowest level elements. Different life cycle stages capture the life cycle of the production alternatives from raw material and utilization to end use.
Second, this presentation demonstrate the empirical results of forest biomass based bionergy production in Eastern Finland that was the topic of recent research project funded by Finnish Funding Agency of Technology and Innovation. The project carried out the comparison of the alternative production chains in the methodological framework described above. The analyzed production chains were as follows: (a) Local heat entrepreneurship based on forest chips (Eno energy cooperative). (b) Wood pellets produced in Finland and distributed to domestic and global markets (Ilomantsi pellet plant). (c) Direct peat combustion in large combined heat and power (CHP) plants (Fortum CHP in Joensuu). (d) Biodiesel produced from both forest biomass and peat (Varkaus experimental plant).
The empirical results of the multi-dimensional comparison of the production chains including economic, environmental, social and cultural sustainability as well as the overall performance when all dimensions are taken into account simultaneously are presented. In addition, the methodological gaps and future development needed are discussed.

LC02B-2
Reducing the carbon footprint of the Swiss energy system: which options are most sustainable?
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One of the main objectives of the research project CARMA (Carbon Management in power generation) is the comparative evaluation of potential options for the reduction of Greenhouse Gas (GHG) emissions from the energy system in Switzerland within the framework of future energy scenarios. This assessment is carried out by applying Multi-Criteria Decision Analysis (MCDA) methodology. The MCDA approach allows considering a comprehensive set of performance indicators addressing environmental, economic and social aspects in decision making and therefore taking into account all three pillars of sustainability; besides these objective criteria, it also allows considering subjective stakeholder preferences, which are used for weighting of the indicators. These preferences are established by a purpose built interactive web interface. The combination and aggregation of performance indicators and preference profiles results in a single performance index for each mitigation option, which can be used for a ranking of these alternatives.
The evaluated GHG reduction options cover the most import economic sectors in terms of GHG emissions: the residential sector, traffic, power generation, and industry. The individual options are evaluated compared to a a kind of "Business-As-Usual"(BAU) reference scenario until year 2050. This BAU scenario assumes a moderate and steady economic growth as well as a slightly increasing population in Switzerland going along with an increase in passenger and freight transport as well as the habitable surface area per capita.
Depending on the indicator weighting profile used for the MCDA - i.e. on the subjective preferences - the comprehensive evaluation of GHG reduction options can lead to different results compared to the most frequently used purely economic perspective. While specific measures are very attractive from an economic long-term perspective, they can lack individual acceptance, or can be associated with high investment costs as a major obstacle to their implementation. Showing the advantages and disadvantages of the evaluated options together with their ranking dependening on subjective weighting profiles in a transparent way can facilitate decision processes and help in understanding barriers in the implementation of effective GHG reduction strategies.

LC02B-3
Evaluating of sustainability as Environmental performance of the regional energy systems
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LC02B-4

Integrating life cycle analysis, human health and financial risk assessment for the evaluation of contaminated site remediation

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When evaluating remediation technologies for contaminated soil and groundwater, the beneficial effect of the remediation, namely cleaner soil and groundwater, are mostly emphasized without consideration of the environmental and social impact of the remediation activities themselves. Nevertheless, practitioners and decision makers can rely on a broad range of decision tools that can help them to achieve a better balance between economic, social and environmental health aspects of contaminated land remediation. A holistic approach for the management of contaminated land should ideally include an assessment of the environmental risk of the contamination, an assessment of the environmental, social and health impact of the remediation process and a cost-benefit analysis of the remediation project.
A life cycle framework, including a life cycle management (LCM) approach structuring environmental activities and life cycle analysis (LCA) for a quantitative examination, can be helpful for the selection of site remediation options with minimum impact on the ecosystem and human health. Besides addressing the environmental impact of the remediation activities for, attention should also be paid to the consequence of reintroducing a remediate site into the economy.
Moreover, certain soil remediation technologies, especially the more 'gentle' remediation technologies are characterized with a lot of uncertainty with regard to the time frame in which the final remediation goals will be achieved. Unexpected situations can result in an increase of the costs of the remediation project. Therefore, there is a need for practical tools that help practitioners in choosing the correct technology that will not only be effective but also will minimize the financial risk associated with the cleanup.
In the present study, several methods that can be used to estimate the environmental, financial and health impact of a soil remediation process were compared. The case studies worked out in this paper want to provide a basis for a more sounded selection of soil remediation technologies based on human health, environmental impact and financial risk criteria.

LC02B-5

Developments in Social Life Cycle Assessment (S-LCA) for Life Cycle Sustainability Assessment (LCSA) - application to the construction and demolition sector in France

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The results of a project aiming at developing a methodology for sustainability analysis dedicated to infrastructures and buildings construction projects will be presented. This research project was carried out in collaboration with ADEME (French agency of environment and energy control), University of technology of Troyes, the Industrial Ecology Club (guild) of Aube and Eiffage (French public works firm). The project is based on a specific case-study concerning the construction of a part of the ring road of Troyes city (Aube, France) where alternative construction materials and techniques, such as secondary raw materials and local natural resources, have been used. A sustainability LCA framework was designed, built on environmental and social LCA methodologies to assess the environmental and social efficiency of such construction projects. It was applied to the case study to compare its global performance with a similar case which would have been conducted in "business as usual"conditions. An environmental LCA was conducted, based on existing international standards. At the same time, a S-LCA methodology was developed on the basis of UNEP-SETAC Guidelines and applied to the French sector of building and construction, to assess social impacts supported by the system's stakeholders. Results showed a high contribution of natural mineral resources use in the total environmental impact, due to extraction and transportation. It was also demonstrated that the energy necessary for asphalt production was much higher than the one for its implementation. Environmental impacts are thus highly dependent on asphalt production and natural mineral resources' quantities and origin. Regarding social impacts, specific impacts categories, indicators and data were searched for and an impacts screening was conducted. Based on sectorial data, it focuses on two stakeholders' categories: workers and local communities. Final results highlight the fact that S-LCA needs strong methodological developments to address intra Europe comparative case-studies and to produce methodologies for system definition, data inventory, impacts characterization, reference databases and specific indicators.

LC02B-6

Life cycle costing of farm milk production - cost assessment of environmental impact mitigation strategies

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Agriculture is a significant contributor to environmental impacts. A study by the University of Arkansas [1] showed that 70% of the carbon footprint of US milk occurs at or before the farm gate. Agriculture is also one of the main contributors to water use and land use, as shown by an ongoing comprehensive milk life cycle study (University of Michigan, 2011). The goal of this presentation is to add costs to the LCA study to determine the impact of the farm milk production system on both the environment and production costs using the same boundaries.

Results and discussion

Three case studies were carried out to compare scenarios from a cost and environmental viewpoint.
The first case study describes a change of manure management system to a digester. For a pilot farm located in upstate New York, the global breakdown of the different processes was assessed both in terms of carbon footprint and production costs Change in GHG impacts and costs are assessed in parralel. Discussion on sources of revenues depending on farm state's location are also discussed.
The second case study compares the cost and environmental impacts of the production of corn, which is one of the major dairy feeds. The costs and impacts (water and land use) are quantified in 3 cases in a sample US state: rainfed, gravity irrigation, and pivot irrigation. This case study provides perspective on how best to represent the costs and revenues, Trade-offs between yield and environmental impacts are also discussed.
The third case study focuses on energy saving on the farm, for a pilot farm in upstate New York. It analyzes the breakeven point, both in term of greenhouse gas emissions as well as in terms of costs.

Conclusion

This study couples environmental impacts and costs, providing a general approach to improve the environmental footprint of milk production on a large range of impacts (GHG, water use, land use) with a measure of the financial costs or benefits of production changes.

LC03 - Increasing scientific and policy understanding through meta-analysis of life cycle assessments

LC03-1

Clarifying estimates of life cycle greenhouse gas emissions from electricity generation technologies: the LCA harmonization project

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Thousands of LCAs of electricity generation technologies have been published. Quality of these studies has varied considerably, as have reported estimates of life cycle GHG emissions. We have completed a systematic review of this literature that included: exhaustive identification and collection of English language LCAs of electricity generation technologies with no bias toward publication type (journal article, report, conference paper, thesis); and multiple, independent reviews of each candidate reference by an interdisciplinary review team that met regularly to ensure consistent screening based on quality of LCA methods, completeness of reporting and modern relevance of evaluated technology.
Estimates varied mainly owing to differences in assumptions of key parameters. It is possible to adjust previously published LCA results to use more commensurate input assumptions and system boundaries, a process we call 'harmonization.' We harmonized estimates of life cycle GHG emissions for six categories of electricity generation technologies: coal, natural gas, nuclear, wind, photovoltaics (crystalline silicon and thin film), and concentrating solar power. While this process is not a formal sensitivity analysis, it does suggest which are the key parameters influencing life cycle GHG emissions for a given technology, such as thermal efficiency for combustion systems, solar resource for solar technologies, and capacity factor for wind turbines, amongst others. Harmonized estimates of life cycle GHG emissions compared to published estimates generally reveal a significant reduction in range and interquartile range from harmonization and often, but not always, an unchanged estimate of central tendency (median). In this way, harmonization is shown to be a method that can reduce variability and clarify central tendency of estimates of life cycle GHG emissions of electricity generation technologies in ways that are useful for policymakers and analysts. Given tight harmonized distributions of a large number of estimates, it is concluded that new LCAs of many technologies (e.g., onshore wind, pulverized coal) are not necessary for the purposes of broad policymaking and first-order analyses, while knowledge gaps or uncertainty remain issues for several other technologies (e.g., natural gas, deep offshore wind).

LC03-2

Meta-analysis of life cycle analysis studies on electricity generation with carbon capture and storage

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Currently, electricity generation contributes to 40% of global carbon dioxide (CO2) emissions. Carbon capture and storage (CCS) technology is widely recognized as an

appropriate option to achieve ambitious CO2 reduction targets. In the last decade, numerous life cycle assessments (LCA) on environmental impacts of electricity generation with CCS have been conducted. This meta-analysis comprises fifteen LCAs of the three CCS technology routes (post-combustion, oxyfuel, pre-combustion) for greenhouse gas reduction for different regions (Europe, United States, Japan, global), different fuels (hard coal, lignite, natural gas), and different time horizons (between present and 2050). The goal of this meta-analysis is to provide a structured overview of assumptions and methodological choices made and, where possible, their effects on the outcomes. The study answers three key questions: 1) Is LCA an appropriate method to evaluate the environmental effects of CCS, and with what validity or limitations?; 2) Is it possible to draw general conclusions regarding the environmental performance of CCS power plants compared to power plants without CCS from the existing LCAs?; 3) Do certain trends arise across the different capture routes or fuels used?
All LCAs show reduction in global warming potential but an increase in other impact categories, regardless of capture technology, time horizon, or fuel considered. Three parameter sets have a significant impact on the results: 1) power plant efficiency and energy penalty of the capture process, 2) CO2 capture efficiency and purity, and 3) fuel origin and composition. However, the normalization indicates only a small impact from CCS power plants on total global environmental impacts.
The meta-analysis proves that LCA is a helpful tool to investigate the environmental consequences associated with CCS. Differences in the underlying assumptions of the LCAs as well as methodological shortcomings yield in heterogeneity of results. A sophisticated and common understanding of the most important technological parameters is necessary to draw a clearer picture of both single CCS techniques and comparisons across techniques. Therefore, it is essential that LCAs include well documented parameters and describe uncertainties and assumptions precisely. There also remains a wide field of subjects and CO2 capture technologies of 2nd generation (like membranes) that have not been covered yet.

LC03-3
Simplified life cycle approach: GHG variability assessment for onshore wind electricity based on Monte-Carlo simulations
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The environmental impacts of electricity production systems have been widely assessed over the past years with many published LCAs in the literature. In the special case of greenhouses gases (GHG) from wind power electricity, the LCA results variability observed is very high, for example ranging from 2 to 81 g CO2eq/kWh in a literature review performed by the IPCC in 2011. Such result might lead policy makers to consider LCA as an inconclusive method. For environmental impacts from electricity generation this is a senstivive issue.
There is a need for a more comprehensive approach to assess the GHG variability so as to define generic results which meet a general consensus. Different attempts have been initiated in order to address this problematic, the use of meta-analyses in LCA being one of them.
The main objective of this paper is to build a representative model of onshore wind turbines (WT) to assess environmental performances with a simplified life cycle approach. A first methodology to generate simplified models for WT environmental performances has been designed (reported in the special issue of the Journal of Industrial Ecology) and is now improved with a better identification of the GHG variability assessment. Variability of GHG performances of onshore wind turbines, generated for a representative sample, is assessed through the running of Monte-Carlo simulations to identify the key parameters having the biggest influence on the results. Based on these Monte-Carlo simulations, we plotted GHG performances distributions for two key identified parameters: the WT life time and the annual average wind speed. A set of generic GHG performances curves has been defined as a function of these key parameters. Results are ranging from 2.7 to 119.7g CO2eq/kWh, a range which is comparable to the mentionned IPCC litterature review. These results can be adjusted as a function of either one or both key parameters. This methodology will be applied later for all types of electricity generation systems to generate simplifed life cycle approaches.

LC03-4
What can meta-regression analysis tell us about variations in life cycle assessment (LCA) results for greenhouse gas (GHG) emissions estimated for advanced biofuels?
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This paper presents a systematic literature review of LCA studies of advanced biofuels (i.e. biomass-based fuels produced from lignocellulosic materials and microalgae). The main factors influencing LCA study results are characterized and estimated using a meta-regression analysis in order to clarify conclusions about their environmental performances. LCA has been widely applied to calculate the Global Warming Potential (GWP is an impact indicator for GHG emissions) associated with biofuel life cycle. Those LCA results can vary significantly depending on various factors: assumptions at biomass production step (N2O emission estimations, inclusion of direct and indirect Land Use Change-LUC), data for biomass conversion into biofuel and general LCA methodological choices (system boundaries, coproduct impact accounting, etc.).
Here, we propose an alternative approach to previous narrative surveys of biofuel LCA studies using the meta-regression analysis methodology to describe and synthesize existing estimates of the GWP of advanced biofuels. It allows to compare and/or combine outcomes of different individual empirical studies with and without similar characteristics that can be controlled for. A database has been built containing a vector of previous studies estimates of GWP (GHG emission indicator expressed in mass of equivalent CO2 per megajoule of biofuel) that has been chosen as the dependent variable of the model since GHG emissions reduction is the most important environmental criteria in regulatory texts, and a vector of explanatory variables. These are factors that can influence LCA results and some study characteristics. Advanced biofuel LCA results from peer reviewed articles, research reports (grey literature) and regulatory texts (RFS and RED) are included in the database (43 LCA studies, 585 estimates). Preliminary results show, ceteris paribus, that the mean life cycle GWP associated with 1 MJ of ethanol, BTL and algae fuel are 27, 21 and 83 gCO2eq respectively (RED fossil fuel reference value is 83.8 gCO2eq/MJ). The analysis shows that GWP estimates are higher in studies that take into account estimate uncertainties, LUC, infrastructures in system boundaries and lower in studies accounting for other impact indicators than only GHG emissions. Moreover, our results indicate that regulatory texts provide lower GHG emissions estimates than peer reviewed studies and that estimates from European studies are statistically higher than American ones.

LC03-5
Sources of variation in life cycle assessments of desktop computers
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Life cycle assessment (LCA) studies of desktop Personal Computers (PCs) are analyzed to assess environmental impact of PCs, and to explain inconsistencies and disagreements across existing studies. Impacts, characterized in this work in terms of primary energy demand and global warming potential, are decomposed into inventory components and impact per component in order to expose such inconsistencies. Additional information from related studies, especially regarding use-phase energy consumption, helps interpret the LCA results. The weight of evidence strongly suggests that for primary energy demand and contribution to climate change, the use phase is the dominant life cycle phase; manufacturing impacts are smaller but substantial, and impacts due to product transportation and impacts due to end-of-life activities are much smaller. Each of the few LCA studies that report manufacturing impacts as being greater than use-phase impacts make unrealistically low assumptions regarding use-phase energy consumption. Estimates of manufacturing impacts, especially those related to printed circuit boards and integrated circuits, are highly uncertain and variable; such estimates are very difficult to evaluate, and more systematic research is needed to reduce these uncertainties. The type of computer analyzed, such as low-power light desktop, or high-power workstation, may dominate the total impact; future studies should therefore base their estimates on a large sample to smooth out this variation, or explicitly restrict the analysis to a specific type of computer.
This abstract is based on a journal paper currently in press with the Journal of Industrial Ecology, due to be published in early 2012 in a special issue on meta-analyses of life cycle assessments.

LC04 - Latest developments in uncertainty management - adding value to LCA studies

LC04A-1
Quantification of uncertainty and spatial variability of characterisation factors in the new global LCIA method IMPACT World+
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IMPACT World+, a new LCIA method representing an update of the IMPACT 2002+ LCIA method, was developed as a regionalised methodology covering the entire global scale, and including uncertainty information encompassing spatial variability and model uncertainty. Up to now uncertainties were only quantified in life cycle inventory databases, notably ecoinvent. IMPACT World+ now provides quantitative uncertainty estimates for each characterisation factor (CF) and thus allows for a complete uncertainty analysis for an entire LCA study. This presentation introduces the approaches used to estimate, quantify, and combine uncertainty and spatial variability for CFs in each impact category. The uncertainty and spatial variability are quantified and kept separately, allowing for differences in spatial variability of CFs in different spatial scales (e.g. watersheds for water use impacts, biomes for land use impacts, and urban/rural archetypes for respiratory impacts, or soil and water archetypes for metal toxic impacts compared to a global or continental average CF. This results in two semi-quantitative pedigree-matrices, per impact category respectively representing uncertainty and variability. Assigning a GSD2 to each of the five uncertainty/variability classes ranging from “no”to “very high”uncertainty/variability allows translating the qualitative into quantitative information. The resulting GSD2 values for the identified main coefficients that compose the CF, e.g. for human health iF, dose-response, and severity factor, can then be combined into a total GSD2 for each CF. A pragmatic and operational solution was required to provide estimates for characterisation factors that count from a handful in some impact categories such as Eutrophication to up to thousands for human health or ecotoxicity. IMPACT World+ is the first LCIA method to provide

quantitative uncertainty for each CF using an estimation framework that is consistent with life cycle inventory uncertainty estimates from e.g. ecoinvent. Given the various types and sources of uncertainty contributing to the overall uncertainty of a CF, the estimates provided are not covering all uncertainty sources and types, and might have a somewhat limited accuracy. They are however an important operational starting point to consistently apply uncertainty analysis in LCA, ultimately allowing to quantify the confidence in LCA results and hence the related conclusions and decisions.

LC04A-2

Quantification of uncertainty of characterisation factors due to spatial variability

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Except for a minority of foreground production sites, elementary flow geographic location is only known to the country resolution. More precision is needed to pick the right spatialized characterisation factors (s-CF) from a set. Countries are usually covered by several s-CF, and their value might span over several orders of magnitude. So far, this source of variability has not been quantified. This paper presents a general method quantifying the uncertainty created by the dichotomy in spatial resolution between inventory and impact assessment.

For each country, a generic CF (g-CF) has to be calculated with the s-CF covering it. Two elements are necessary to build the g-CF: the probability density function (PDF) of each s-CF, and a set of weighting factors. The weighting set provides a likelihood of emission on the zone covered by each s-CF, an information lacking in the generic unit processes. The average and standard deviation of the g-CF is not calculated directly from the weighted s-CF. Instead, the PDF of the g-CF is built by adding the weighted PDF of each s-CF. The average value of the g-CF can be calculated from the PDF and used in deterministic calculations. The standard deviation could be useful if the resulting PDF can be approximated by a normal or lognormal. Otherwise, the full PDF should be reported and used directly in a Monte Carlo simulation.

Finally, the coefficient of variation (CV = average/standard deviation) of the g-CF can be compared to the CV of the s-CF. The CV of the g-CF will be higher, and this augmentation of uncertainty reflects the spatial variability that cannot be taken into account, due to the lack of spatial information in the generic unit processes.

The impact category chosen to demonstrate this methodology is water use on human health. The spatial delineation of this method is the intersection of countries and watersheds, resulting in 808 cells. The likelihood of water use in each cell is based on data from the Watergap model. China is covered by 20 watersheds. The corresponding 20 s-CF are lognormally distributed with CV between 0.6071 and 0.6218. After adding their weighted PDFs, the resulting g-CF is bimodal, with a CV of 7.63. This means that if a use of good quality water occurs somewhere in China, without further information on the watershed of consumption, it will be characterized with a g-CF of a value potentially much greater or lower than with the right s-CF, and roughly 10 times more uncertain.

LC04A-3

Matrix-based sensitivity and uncertainty assessment for evaluating human intake of pesticide residues in food

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Multiple pathways contribute to human exposure towards pesticides: inhalation after air emissions, ingestion after soil and water emissions and, most importantly, ingestion of directly sprayed food crops. For the latter, we developed a dynamic multicrop model for assessing pesticide residues in food crops and subsequent human intake. However, full uncertainty analysis is still lacking. We already identified half-lives in plants and time between substance application and crop harvest playing a crucial role, but other aspects may also be important.

We designed a simple but accurate regression model with time from application to harvest, half-life in plants, residence times in the environment and key substance properties as influential input variables. Additional influences are identified by assessing relative sensitivities of a wide range of input variables, thereby addressing parameter correlations and defining geometric standard deviations for all relevant input variables as a function of their base uncertainty and spatial/temporal variability.

We studied the uncertainty propagation of the model outputby applying a new approach of calculating the overall output uncertainty as a function of the matrix of relative sensitivities of input variables and the covariance matrix expressing their correlations. Model output, i.e. human intake fractions from consumption of food crops treated with pesticides, showed highest relative sensitivities across substances to half-lives in plants and on plant surfaces as well as to the time between substance application and crop harvest. Total output sensitivity is a function of the crop species and is highest for leafy vegetables (lettuce) and fruit trees (apple). We also studied the variability across pesticides, from which we derive crop-specific regression models predicting residues in food crops across pesticides within a factor of 10 of those calculated with the complex model as a function of only a handful of input variables. These simplified models are adequate to assess direct residues for multimedia models used for risk and impact assessment and, hence, enable the user to calculate direct pesticide residues by only providing a very limited set of input information.

LC04A-4

Uncertainty classification and implementation in life cycle impact assessment: application to freshwater ecotoxicity of pesticide application to Maize in The Netherlands

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How to deal with uncertainty has become a key challenge for integrated assessments. As yet, the application of an uncertainty analysis is not common practice in life cycle assessments. A proper analysis will be facilitated when it is clear which types of uncertainties exist The aim of this research is to set up a framework to classify levels of uncertainty in life cycle impact assessment (LCIA) and demonstrate the practicability of the framework with a case study example on freshwater ecotoxicity caused by pesticide application in The Netherlands.

Three levels of uncertainty were distinguished. (i) Statistical uncertainty, arising from measurement errors, analytical imprecision, and limited sample size; (ii) Decision rule uncertainty, caused by ambiguity or controversy about how to quantify or compare social objectives; (iii) Model uncertainty, defined as uncertainty about the relations and mechanisms being studied. To quantify statistical uncertainty, uncertainty distributions need to be derived for input parameters and propagated to output uncertainties, e.g. via Monte Carlo simulation. Decision rule uncertainty and model uncertainty can both be made operational with the help of a choice analysis.

A case study that addresses the application of pesticides to maize in the Netherlands was performed to show the application of the various uncertainties for freshwater ecotoxicity. Statistical uncertainty in freshwater ecotoxicity damage scores was quantified by performing a Monte Carlo analysis with chemical-specific input parameters set as uncertain. Decision rule uncertainty was determined by identifying choices in the damage quantification, i.e. availability of toxicity data, choice of effect factor model (linear or non-linear), and the damage factor (modeling up to midpoint or to endpoint). Model uncertainty was quantified by including and excluding pesticide transformation products.

Results showed that damage can vary substantially depending on the value choices made. Parameter uncertainty can increase to a large extent when a more accurate model is applied. Going from midpoint to endpoint applying an uncertain damage factor decreases the damage slightly, but hardly changes uncertainty. Only when transformation products are included, going form midpoint to endpoint increases median damage clearly.

LC04A-5

Data quality metrics in Life Cycle Impact Assessments: application to a case study of cellulosic biofuel

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Although guidelines exist for assessing data quality in life cycle impact assessment (e.g., ISO-1404), they are seldom implemented satisfactorily in practice. A need therefore exists for transparent, consistent, and credible data quality metrics that facilitate the prioritization of data needs and enhance the reliability of LCIAs. Monte Carlo (MC) methods, such as sensitivity and uncertainty analysis are used to identify the most influential inputs and to understand how input uncertainty (variability and lack of knowledge) is propagated through to the calculation of output metrics. However, MC methods are rarely applied in LCIAs. Here we demonstrate the application of sensitivity analyses coupled with a data quality evaluation scheme, to assess uncertainty in output metrics in our LCA "Carbon Tool", which quantifies the environmental and human health impacts associated with national-scale cellulosic biofuel production. Programmed in Excel, the Carbon Tool estimates environmental and health impacts associated with biomass, biorefining, and transportation stages of biofuel production. Specific output metrics include: greenhouse gas emissions (fossil CO2, and GWP100), total energy, and human health impacts associated with criteria air pollutant emissions. We use the Spearman rank correlation coefficient to identify influential variables for each output metric, with specific application to Miscanthus ethanol production. We then evaluate the uncertainty in influential system variables, using a qualitative data quality evaluation scheme adapted from Junnila and Horvath (2003). Of the eight variables evaluated, Combined Heat and Power (CHP) penetration was the most influential system variable on the total energy and fossil CO2 output metric. However, the "CHP penetration"input ranks low in terms of the geographical correlation and overall representativeness, and is based on assumptions (low rating for data acquisition). For human health impacts, specifically those for PM emissions, the three most influential system variables are associated with truck and rail distance traveled. But, the data for these inputs rank low in terms of temporal, and geographic coverage and are based primarilty on assumptions (medium rating for data acquisition). We find that our data quality framework, coupled with MC methods, can help prioritize data collection efforts to focus on those inputs that significantly influence the outcome metrics, and have low data quality ranking.

LC04A-6

Uncertainty analysis in macro-level life cycle assessment

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Developments in life cycle assessment (LCA) have led to new life cycle thinking applications such as the macro LCA approach (M-LCA), an extension of consequential LCA (C-LCA) that implements elements of prospective LCA in order to model medium- or long-term environmental impacts related to global economic perturbations caused by major changes occurring in multiple life cycles. In M-LCA, economic impacts are based on the GTAP model, an economic general equilibrium model (GEM), which provides the production variations for each economic sector in each region of the world in response to a given economic change. The environmental impacts of each regional economic sector are then computed according to the LCA methodology. As uncertainty related to GEMs and LCAs is recognized as significant, the uncertainty associated with M-LCA is expected to be as well. For this reason, an uncertainty analysis was conducted on an M-LCA comparison of two European Union (EU) energy policies (business as usual vs. bioenergy). Uncertain exogenous variables and internal parameters used by GTAP were combined in order to develop 27 scenarios that were run in GTAP to define a tree of potential economic consequences caused by each EU policy under the assumption of each scenario. Environmental impact uncertainty for the 27 scenarios was then assessed using a Monte-Carlo (MC) analysis. Results of the uncertainty analysis show the M-LCA comparison of EU policies is not sensibly affected by uncertainty for climate change and natural resources while the comparison is more uncertain for human health and ecosystems. The uncertainty analysis also highlights that several sources of uncertainty in M-LCA cannot be assessed due to lack of information on data uncertainty (external data used for the linkage of GTAP and LCA databases and forecasts used to model the evolution of temporal variables) and the difficulty in comparing GTAP results with historic data. Additionally, it appears MC analysis is not adequate to study uncertainty propagation in complex models such as M-LCA. Indeed, due to the significant quantity of uncertain parameters, the time required to conduct the MC simulations makes this approach unfeasible without extensive computational resources. Therefore, the development of another approach based on an uncertainty management method more suitable for large models, like Gaussian quadrature or Fourier transformations, would improve the management of uncertainty in M-LCA.

LC04B-1

Technological, geographical, time-related uncertainty measurements for textile spinning and weaving processes

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Life Cycle Assessment (LCA) is very dependent on the quality, relevance and reliability of the Life Cycle Inventory (LCI) data sets selected by the LCA-practitioner. When modeling a system, the representativeness of the LCI data set is complemented by the appropriateness of the data set in the context of the specific system. The appropriateness characterizes, in how far a data set in a system model represents the truly required process or product. According to the ILCD handbook [1], the use of not fully appropriate data is justifiable only if this is not relevantly changing the overall LCIA results compared to using fully representative data; otherwise the lower achieved representativeness shall be documented in the report. But when the required data is missing the practitioner has limited possibilities to evaluate any differences between the required data and the available data.
This paper aims at evaluating the appropriateness of different LCA-practitioner choices regarding the geographical, technological and time related representativeness in the modeling of a product life cycle. The examples are taken from two technologies from the same industry domain that behave differently and require different LCA methodologies.
First, different LCI data sets for spinning and weaving processes in the textile industry are inventoried. The precision, completeness, representativeness and methodological consistency of these LCI are briefly described. Then, the following data quality tools: gravity analysis and sensitivity analysis [2] are applied at the assigned LCI results. The gravity analysis reveals the main contributors to indicator scores. The sensitivity analysis measures the change in the indicator results for induced changes in LCI results. Practically, the LCI results for different geographical situations, for different technologies (time related or not) and for different scenarios (average world scenario and worst case scenario) are compared.

LC04B-2

A comparison of uncertainty propagation methods in an LCA study

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Several methodologies can be used for defining and propagating uncertainties affecting model input data in LCA studies, according to the nature of available information. Probability theory is the most commonly used and consists in defining uncertainties as single probability distributions and then propagating them through stochastic modelling or analytically. For cases where available information does not justify the use of single probability distributions for representing uncertainty, possibility theory provides an alternative method which consist in defining uncertainties as fuzzy sets.
The objective of this paper is to illustrate the fundamental differences between these approaches using on the one hand classical stochastic modelling, fuzzy calculus, and finally a hybrid method which combines both approaches. In this last method some parameters are represented by single probability distributions (because they are justified by available data) while others are represented by fuzzy sets (because available data is incomplete and/or imprecise). The joint propagation of these different modes of uncertainty representation was performed using the independent random set method proposed by [1].
The case study investigates the benefits of sending the organic fraction of household waste to anaerobic digestion instead of incinerating it, in Danish conditions. For each chosen parameters, data was gathered through a litterature review to define the uncertainties underlying each parameter, using either a single probability distribution representation, or else a fuzzy-set representation.
Comparison between the three propagation methods illustrates the very conservative nature of the purely fuzzy calculation, of which the result of the stochastic calculation is but one representative among others. Results of the hybrid calculation on the other hand are more precise than the fuzzy calculation but of course less precise than the purely stochastic result which assumes that single probability distributions are perfectly known for all input parameters.
In real-world situations of LCAs, available data are typically of different natures. Therefore the proposed method can serve to jointly propagate the different types of uncertainties in the LCA.
[1] Baudrit, C., Dubois, D., Guyonnet, D., 2006. Joint propagation and exploitation of probabilistic and possibilistic information in risk assessment models. IEEE Transactions on Fuzzy Systems, 14 (5), 593-608.

LC04B-3

The impact of processing natural resources on uncertainties in life cycle assessment

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Natural resources are often connected to variable compositions. Ore from mining operations seldom provide the same ore concentration of their production everyday and the further processing has to deal with it. The same effect is visible in renewable material flows like wood, gras, and crops for example. By processing these materials the process has to be either adapted to the changing quality of input material or it is run on average level. An average process control level may have an inefficient effect on the process quality.
This presentation will concentrate on the question: How to run a material and energy efficient production process with less environmental impact? Our study case is the production of pig feed in a commercial feed processing plant in Northern Germany.
Our aim is to relate the energy consumption not only to the process steps but to the various recipes. By identifying the carbon footprint for each recipe we are going to optimize the energy input into the process without influencing the product quality. This is our highest challenge, since the quality of the end product cannot be changed due to the animals demand.
This can be achieved by monitoring the process by online measuring systems and developing an expert system that is able to control the process by using fuzzy rules. The definition of the fuzzy rules are dependent on the identified uncertainties within the process. During the handling of renewable materials uncertainties can be found in their composition due to the fact that we are handling natural resources with varying properties like their water content for example.
The uncertainties in feed processing can be divided into:
- uncertainties that can be influenced by the process control (adjusting the water content by adding water)
- and uncertainties that can not be influenced by the process control (chemical composition)

The development of the expert system of the production process (case study pig feet) is performed according to uncertainty management. Uncertainties are present at any time in the process and has therefore taken into account during the decision making process. In the end it will be possible to simulate the production process with varying parameters to evaluate the result of the simulation. This helps in assessing the process set up and in logistics question (what is the best cyclic order of the recipes to consume the least energy?).

LC04B-4

Introducing an uncertainty analysis methodology, in an international carbon footprint accounting for decision making, Renault Group case study

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Climate change and energy dependence are major challenges for the transport industry. Tackling these requires major decisions and therefore to integrate Greenhouse Gases

(GHG) management in companies. The two first actions to go through are accounting over the complete life cycle and involving all the employees and key stakeholders in the progress. Due to the breadth of the approach, it is of utmost importance to evaluate uncertainty in order to ensure the best decision-making.
The hybrid product/organisation accounting method is based on the product Global Warming Potential calculated and reviewed according to ISO LCA norms. LCA often neglect employee mobility and workplace behaviour. Therefore these items are added according to the GhG Protocol.
Interpretation of the results is crucial and a specific uncertainty analysis method has been developed. Uncertainty is analyzed separately for Physical Input (PI) data and Emission Factors (EF). The pedigree matrix takes into account reliability, completeness, and temporal, geographical and technological representativeness of data according to five different quality levels. Accuracy is increased by introducing a specific factor for the availability of Physical Input primary data versus secondary. Finally Emission Factor quality are specific of industrial activity. The uncertainty factors are used together to evaluate the global uncertainty.

The majority of the carbon footprint (85%) calculations are in the "good"level, while 10% are of "middle"uncertainty and finally 5% are evaluated as "very good".
When making a decision, it is important to allocate budget toward the most important topics. This uncertainty approach enables deciders to choose under the best conditions. The risk factor can be considered in decisions, helping us to evaluate and improve the inventory each year.
All uncertainty factors are based on Renault expert judgment and should be challenged by external expert (eg. Quality of background LCI database).
Implementing Carbon Footprint accounting is a major step towards an Environmental Footprint management by introducing the life cycle perspective and involving the whole company.
Nevertheless such a wide perimeter implies a complex calculation protocol and the uncertainty calculation will have a huge importance to tackle the complexity of this management and implement the best decisions.
Finally, the authors stress that even if uncertainties exit, these shall not be a barrier for taking action.

LC04B-5
Uncertainty and variability in the carbon footprint of U.S. coal-fired power production
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The overall carbon footprint of power generation can be calculated using life cycle assessment (LCA). For most LCAs, average conditions are used to estimate the environmental impacts of a process or product. However, regional and technological differences in product manufacture, use, and disposal may cause a specific life cycle impact (e.g. GHG emissions) to be lower or higher than that of an "average"life cycle. Moreover, uncertainty in process data used to model life cycle stages may affect the accuracy and precision of life cycle impact assessments. Whereas uncertainty is defined as lack of knowledge and can potentially be reduced by additional research, variability is an inherent characteristic of supply chains and the environment and cannot be reduced.
The aim of this study is to quantify the contributions of uncertainty and variability to the range of the carbon footprint associated with coal-fired electricity production in the U.S. We quantified the effects of spatial and technological variability upon the life cycle emissions e.g. distances between coal mines and the power plants they supply and power plant efficiency. We also characterized parameter uncertainty, e.g. the methane emission associated with a coal basin. The LCA included three stages: mining, transport and power generation, and utilized a functional unit of 1 kWh of electricity generated at the plant. Parameter uncertainty was quantified via Monte Carlo simulation, whereas variability was taken into account via the efficiencies of power plants and coal transportation receipts reported by the U.S. EIA.
We present the individual carbon footprints for U.S. power plants with uncertainty ranges. Our results show that the variability in electricity plant efficiencies particularly lead to a large overall variance of the life cycle emissions of coal power. Results indicate that improvements in inventory data and assessment parameterization reduce the variance of the life cycle emissions. The results can be used to assist decision-makers in ranking the carbon footprints of coal plants and facilitate the comparison of coal power emissions with other power generating technologies on a statistical basis.

LC04B-6
A protocol for approaching uncertainties in life-cycle inventories Monte Carlo analysis - a practical example using aquaculture feeds
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Although LCI values often are presented in absolute numbers, uncertainty and variability are common traits of both foreground and background data. Uncertainties result from limited temporal, spatial and technological coverage of both economic and environmental flows, with a direct influence on results. In LCIs of food production system, however, the influence of variability (ontological uncertainty) may be increasingly predominant as production is governed by natural fluctuations (e.g. yields). Outcomes of LCA results describing the same production system may therefore vary with up to an order of magnitude.
Aquaculture feeds are here used as a practical example to demonstrate the proposed approach to uncertainties in LCIs. The modelling includes foreground data collected from feed mills in Asia and literature sources, while background data derive from the ecoinvent v 2.2 database. Each processes within the system boundary was approached using a standardised protocol to assign mean, standard deviation and distribution to most economic and environmental flows. Each of these variables were based either on primary data, weighted averages derived from a meta-analysis or a numeral unit spread assessment (NUSAP) pedigree. The inventories were later simulated using a Monte Carlo analysis to generate confidence intervals for individual flows.
Using relevant up-to-date inventories is crucial for achieving accurate results and taking uncertainty into account is the only way to justify these results. We, therefore, herein present a practical way on how to consistently source and analyse inventory data using a mix of real values, weighted averages and NUSAP estimations. This allows for a wide range of data sourcing and a constructive strategy for highlighting areas of great uncertainty and identifying data gaps.

LC05 - Monetisation for weighting and aggregation in Life Cycle Impact Assessment and Cost-Benefit-Assessment

LC05-1
Development of national average weighting factors in LIME2 - Visualization of the variability of external cost using statistical analysis
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Recently several methods of economic evaluation have been published in the scientific literature increasing the credibility and the review process. Examples of more recent methods are methods based on monetary valuation of endpoints (Itsubo et al., 2004; Weidema, 2009), the Ecotax method based on a monetary valuation of midpoints (Finnveden et al., 2006), and panel methods for midpoints (Soares et al., 2006; Huppes et al., 2007). Methodological aspects of weighting methods are also reviewed and discussed by (Ahlroth et al., 2011, Mettier and Hofstetter, 2005).
The results are not only easy to understand but can also be used for cost-benefit analysis. While the best way to allocate economic values to environmental impacts such as a loss of health or a decline in biodiversity is still in the development stage and has not yet been fully established.
This study summarized a result of development of national average weighting factors with visualizing of the variability of external cost using statistical analysis. Conjoint analysis was applied to weight across several safeguard subjects and random parameter logit model was adopted to measure the confidence interval of external cost.

LC05-2
Environmental damage cost factors per functional unit of transport activities, heat & electricity generation in Germany
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For decision support, results of LCA often have to be weighted to allow aggregation of impacts and evaluation or ranking of alternatives. Impacts can be expressed in monetary terms to facilitate appropriate taxing or subsidies, and cost-benefit-analysis, etc. If impacts on human health and the environment are expressed in monetary terms they are called environmental damage costs (EDC). The share which is not internalised into economic decisions is called external costs. Starting in the 1995, within the ExternE (External Costs of Energy) project-series methods for estimating EDC have been developed. The methodology has been further improved in several EU-projects. In 2011, within a project for the German Federal Environment Agency, cost factors have been re-calculated for different transport activities, heat & electricity supply in Germany including operation and up- and downstream processes, also outside Germany. A large amount of results is available providing differentiation between energy carriers and technologies for heat and electricity. Moreover, with regard to transport activities different energy carriers, modes and different technologies have been assessed. Results are available at www.ExternE.Info.
The updated and extended impact pathway approach provides results which are more reliable and conclusive as it combines site specific assessments, as far as possible, but also includes average values for different source characteristics and regions.
The uncertainties due to spatial variability inherent in many LCIA methodologies are transparent because country specific values are further differentiated into sub-regions, urban and rural environment, and different heights of releases. The results can be used to support decision making, perform cost-benefit-analysis and test more simplified approaches in the future.

LC05-3

Comparative LCA of potable water production plants using economic valuation

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In potable water production, the question of finding a fair trade-off between the water quality increase, from raw water to at least the potable water standard, and the total effort to be spent to reach that objetive is very common despite not trivial. Few comparative LCAs of potable water plants have been published, mostly disregarding the water quality increase in the functional unit and therefore obtained erroneous conclusions. Water quality gain (WQ) can be evaluated by using water quality indicators as the Quality Valuation System for Water (SEQ-EAU in French), further aggregated into a single score through a statistical approach. Regarding the total effort spent to reach the gain (TE), monetisation of LCIA results (Stepwise2006 and Eco-costs2007) is indeed a very effective and practical approach, as compared to traditional single scores like ReCiPe, to obtain a single numeraire, which can be further combined to the total operational costs of the water treatment plants to be fully understandable by investors and decision makers. In the framework of an international research project, we developed a novel performance index (PI), defined as the ratio WQ/TE, which allows to properly compare alternative potable water production plants. Statistical tests are used to get a confidence interval for the PI of each plant but also for the difference of the PIs between plants. The PI was applied on two existing treatment plants managed by Suez Environnement in France. The plant comparison using the PI calculated with ReCiPe is not conclusive, since the confidence interval of the difference of the average PIs includes zero (too high uncertainties). The same evaluation with monetized scores, augmented by operational costs, gives a clear preference for one of the two site. Further research is ongoing to add infrastructures data in the LCIA calculations and to implement LCIA uncertainties into the performance index.

LC05-4

Development of an integrated indicator for land use based on ecosystem services

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In life cycle impact assessment (LCIA), potential impacts due to land occupation are calculated with the equation: $I_{occ,i}$ = surface * $time_{occ}$ * ΔQ_i. Currently, the only i indicator for the land quality loss ΔQ_i is related to terrestrial biodiversity (PDF.m^2.year) and is not representative of all impacts, which are described by the European Commission (2010). Recently, an improved land use method has been developed with the UNEP/SETAC Life Cycle Initiative project (LULCIA, 2008-2011). This method relates land use to six new indicators: biotic production (BPP), erosion regulation (ERP), fresh water regulation (FWRP), mechanical and physicochemical water purification (WPP) and carbon sequestration (CSP) potentials, which represent provision and regulation services, as defined in the Millenium Ecosystem Assessment (2005).
While this development improves LCIA methodology, it also reduces the decision support system capacity of LCA, providing seven midpoints for land use alone.
This project aims to develop a new method (factors in $/indicator unit) using economic valuation as a common thread to convert the new indicators to endpoints representing ecosystem services loss (potential damage costs). This conversion also allows aggregating into a single indicator. The values of BPP and CSP are respectively estimated with productivity loss and carbon tax. The other regulation services values are estimated through current compensation costs, as they are considered essential (conservative approach). As a local impact category by nature, spatial variability and the availability of the compensation systems are taken into account. Economic valuation assumptions will be discussed. Finally, this method brings a new level of interpretation and potentially allows LCA to assess other impacts related to land use, such as aesthetics and recreational aspects.
This method will be applied on a case study involving the comparison of production locations for bio-based polymers.

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LC05-5

How to correct price for monetising non-renewable resource consumption?

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Monetising aims at reflecting how human well-being is affected by an activity. This paper focuses on the impact category "Non-renewable resource consumption"(mineral and fossil). The cost for the society of consuming such resources corresponds to the well-being loss due to the increased resource scarcity in the future as a consequence of its consumption today. It can be assessed through the opportunity cost, defined as the welfare loss (the cost) of being deprived of an extra unit of resource for its most valuable use, i.e. the one providing most utility. In a perfect market, the price is optimal as it allows maximising the total welfare provided by the resource (optimal resource allocation). In a more realistic market, the question is: "Does the actual market price need to be corrected for deriving the cost for the society of consuming resources?"The methodological approach developed is based on the following analysis:
- the market price is driven away from the optimal price since, as generally admitted, private discounting rate is higher than social discount rate.
- Other main drivers in market pricing have similar mechanisms in actual and perfect markets and, furthermore, these drivers are better assessed by the market than by a modeller
The developed monetisation factors for non-renewable resource consumption consist hence in using trend market prices multiplied by a factor correcting for the excessive myopia of the market (too high discount rate). The correction factor is calculated using Hotelling's rule to re-discount the projected future opportunity cost at exhaust to a current social cost. For this purpose, market and social discounting rate values are assumed as well as the number of years before the last unit is consumed. A sensitivity analysis on these parameters is carried out. The approach allows obtaining either the whole cost for the society or only the external part.
Main limits are that (i) the correction factor is common to all resources while resources could be classified into different families (ii) the factor is obtained by assuming a partial equilibrium economic model (i.e. effects of potential future internalisation are not taken into account).
In practice, when assessing for example various end-of-life scenarios for electric and electronic waste, the total monetised impacts obtained for all impact categories are often dominated by the contribution due to resource depletion (mineral and fossil).

LC06 - Life cycle management (LCM): Success factors and barriers

LC06-1

Barriers and success factors in the use of LCA and ecodesign tools at Nestlé

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Nestlé, the World's leading Nutrition, Health and Wellness Company, is committed to environmentally sustainable business practices. We assess the environmental impacts of our products using LCA and ecodesign tools. While LCA has been shown to be useful for claims and communication of the environmental performance of our products to third parties and the public, the timeline and cost of conventional LCA is not practical for a widespread application throughout the company.
PIQET, a packaging ecodesign tool, is being used to assess the environmental performance of packaging systems. Its low cost and rapid results generation allow for it to be systematically applied throughout all packaging innovation & renovation projects at Nestlé, creating knowledge on environmental impacts of our packaging and promoting innovation to develop new packaging systems with reduced environmental impacts.
Building on the success factors of PIQET (pre-defined goal & scope and inventory database, simple to use, fast result generation), we have developed a new ecodesign tool that will take into account the entire life cycle of a food product, including the production of ingredients, processing, packaging, distribution, consumer use, and end of life.
To further accelerate the use of such a tool, a link with the company recipe and trial management system has been established. By selecting an existing recipe or trial of a new product from the management system, the ingredients specifications, quantities, and the corresponding processing steps can automatically be uploaded to the ecodesign tool, significantly reducing the manual work required to complete the assessment. By integrating the outcomes of the ecodesign assessment into the stage-gate process for product innovation, a systematic evaluation and optimization of the environmental impacts of all products can be achieved.
For claims and communication of tool results to the public, however, an independent peer-review process according to ISO 14040 & 14044 will still be required. To simplify this process, independently established, internationally agreed LCA and ecodesign methodologies (e.g. the EU Food Sustainable Consumption & Production Roundtable) are used. Furthermore, transparent, independently generated LCI data is incorporated into the ecodesign tool. This reduces the possibility for tool users to introduce bias into their studies and increases the reliability and credibility of the ecodesign tool.

LC06-2

Mainstreaming life cycle management: using a sector based and regional approach in Northern France in the textile, seafood, packaging and mechanical sectors

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Whilst **Life Cycle Management** is becoming commonplace in larger corporations, or forward thinking governments, it is far from mainstream. To achieve sustainable production and consumption patterns, LCM needs to be taken up by whole supply chains that include many **small and medium enterprises**. These businesses typically lack the financial capacity or human resources to implement LC tools on their own, and are wary of working with support organisations outside of their sector or local area.
In Northern France, the **textile, seafood, packaging** and **mechanical** sectors are developing strategic action plans to integrate Life Cycle Approaches (including ecodesign and product environmental labelling) into businesses, education and research organisations. Each study is led by a competitivity clusters or technical centre working within the sector.
The paper will present results of the benchmark of life cycle initiatives and tools relevant to each sector, and assessment of the existing capacity of businesses, education bodies and research centres in the region. Focus will be given to how potential actions are prioritised through engagement with key stakeholders (such as businesses, universities and professional federations) and how this inclusive process maximises with success factors and helps overcome barriers to implementation.
The four action plans are developed in parallel, enabling the sectors to identify cross cutting actions. The paper will explain how this process is managed through a **network of "Life Cycle Champions"**. Champions have been trained in the eight sectors; and meet regularly to exchange experiences in implementing life cycle approaches and identify cross cutting projects. The 4 other sectors will undertake the strategic action planning process in a second "wave", to incorporate learnings from the first process.
This innovative approach to mainstreaming LCM leverages sectorial and regional networks to help overcome barriers to implementation. From a business perspective, integration with existing professional organisations means that SMEs access advice and tools through organisations that they already know and trust. Working with several sectors in parallel through the Life Cycle Champion network encourages a multidisciplinary approach, essential to improving decision making across entire supply chains.

LC06-3
Driving proactively the sustainability agenda for the European detergents and maintenance products industry, via the A.I.S.E. Charter for Sustainable Cleaning
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A.I.S.E., the International Association for Soaps, Detergents and Maintenance Products, has a long tradition of proactive work towards sustainable production and consumption. Its main overall scheme is the A.I.S.E. Charter for Sustainable Cleaning, encouraging the adoption of sustainability management practices at all stages of the product life cycle; launched in 2004 in all EU countries plus Norway, Iceland and Switzerland, the Charter covers all products categories of the detergent, cleaning and maintenance products' industry.
Participating companies report regularly progress on Key Performance Indicators, leading to the publication of an annual sustainability report.
As at November 2011, commitment to the Charter is a success with 160 companies committed, covering approximately 85% of the total industry's production output;
An update of the Charter has been rolled out in summer 2010, introducing a product dimension to the existing Charter requirements. This fits very well with the overall objectives of the European Commission SCP/SIP Action Plan, and particularly the Ecodesign Directive.

LC06-4
Life Cycle Assessment, from an evaluation tool to a collaborative eco-design enabler for electric vehicles
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The automotive industry is facing major challenges and the stress is strong in order to reduce production cost and usage value within the capacity of the nature to support the mobility growth.
This goal will be achievable only when a co-innovative product design will be set up, involving the whole value chain [1]. This is an ambitious target and this paper will show how life cycle assessment evaluation tool could be a major contributor to bring the various parties altogether.

Several example are identified, from the more obvious which is the critical review during which the practionner will open his work to Research Institutes / Universities or Environmental Non-governmental Organizations. Regarding the impact assessment, relaibility can be worked with Research Institutes when comprhension can be studied with Customers. Concerning Inventories employees and suppliers will work hand in hand and finally for the scope definition, this will be a good opportunity to involve the customers in order to define the relevant functional unit. This last point is particulary true when speaking of the electric vehicle, a new technology and potentially a major change in people habits of buying and consuming their mobility.
One result example is the definition of the functional unit for electric vehicles LCA [4]. The main difficulty [5] is to define a function equivalent between thermal and electric vehicles. The ILCD handbook [2] recommends a functional unit define by four items: What, How much, How long and in What way. The reason for any doubt take place in the last item, in what way. This question was studied under two approach, one "product centric"based on functional analysis and one "people centric"based on customer (emotional) needs. Then we can enlight the main differences between the thermal vehicle strengths - reassurance and aesthetic - versus electric vehicles ones - environmental friendly and fun-. Therefore, equivalent functional units shall add a reassurance dimension to the electric vehicle functional unit such as an easy access to a "long autonomy range"vehicle when needed.
This experience on the electric vehicle shows also that LCA can be a very useful tool to bring the stakeholders (unusual ones as NGOs as well) around the table with a positive and constructive scientific approach.

LC06-5
LCT in the floor-covering industry: the strategy of Tarkett
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Tarkett is world-wide leader in innovative flooring and sports surface products, providing integrated solutions to professionals and end-users. Despite its long time concern about environmental issues, actions remained not harmonized so far. The main tool reflecting environmental performances of Tarkett activities and products was the regular publication of five environmental "Key Performance Indicators"on global production. The need for a comprehensive sustainable development strategy to be integrated in the daily practice has emerged and Tarkett is now engaged with a multifold challenge. To tackle this endeavor, Tarkett has chosen the support of the Public Research Centre Henri Tudor. Life-Cycle Thinking (LCT) has been identified as main approach, since the products are at the core of the environmental strategy system. Tarkett deals with a wide range of market segments, 30 worldwide production sites, 8 families of products, and therefore a wide range of raw materials. The implementation of LCA as a fact based practice for process and product environmental improvement has therefore become a priority. Although LCA is used as an eco-design driver and a strategic tool, the company is aware that this tool is not sufficient at its actual level of development to address some specific issues. Therefore Tarkett is engaged in complementary development studies and processes. The adopted approach is a progressive integration of LCA as a decision-making tool in a coherent way for all Tarkett's branches. First Tarkett acquired knowledge on LCA, through training sessions in Europe and the US. Then, systematic LCAs of product families have been realized. Dedicated IT software is also being developed to facilitate the access to LCA models and allow Tarkett professionals to run ecodesign simulations. The positive feedback from this test integration phase convinced Tarkett of the ability and reliability of LCT to drive the implementation of environmental strategy at the decision making level. Further development phase is now launched; the vision is to combine the complementary tools already used by Tarkett in the LCT process, in order to set a robust decision making based on eco-innovation criteria.

LC06-6
Promoting use of life cycle management in Finnish companies - challenges, benefits and suggestions for future value networks
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Life cycle thinking (LCT) and life cycle assessment (LCA) along with other life cycle (LC) methods are important tools in assessing environmental impacts of products and services, and to support environmental decision making in companies. Use of those methods can also help companies to find out business opportunities by taking precautionary actions. This study presents the main drivers and barriers for companies to apply LCT, LCA and other LC methods. We also suggest a roadmap for the promotion of these methods in companies and their value networks. We first assessed the methodological challenges of the LCT, LCA and other LC methods from the company perspective. The applicability of those tools was assessed in several case studies. The assessments were based on the data from literature and companies. Several stakeholder workshops were organized to get practical views on the use of LC methods. The current and future use of LC methods in companies was also studied using an internet questionnaire and thematic interviews. They revealed that the companies can coarsely be categorised in four main company types regarding their knowledge, resources and potential to utilize life cycle methods in practice. The findings were supported by the case studies. Three company types were named as 'interested outsiders', 'learners' and 'forerunners'. Additionally a large group of companies are not aware of the use of life cycle methods and their potential benefits. The main drivers for the environmental management of companies included legislation requirements, improvement of cost-efficiency and customer requirements, among others. A large number of

companies are not familiar with life cycle methods and their potential benefits. Additionally, especially of small and medium-sized enterprises (SMEs), often have no temporal, human and economic resources to learn and educate themselves on the benefits of using LCT and LCA. The main challenge related to wide use of LCT and LC methods in companies is probably related to the communication problem between the LC researchers and companies, and therefore much more practical approach need to be used when spreading LCT in wide scale. The next step in promoting the use of LCT and LC methods in decision making in practice will be a pilot project, in which all the actors within a region, value-chain or sector will be introduced to work with each others in to a networking process, including special type of training for SMEs.

LC07 - The UNEP-SETAC Life Cycle Initiative: a decade of supporting the global LCA community

LC07-1

Scientific legacy of the UNEP-SETAC Life Cycle Initiative: contributions and significance

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The UNEP-SETAC Life Cycle Initiative is a joint venture formed in 2002, among several purposes, to foster the development, validation, and dissemination of methods, tools and practices for lifecycle assessment and management. Over its ten year history the Initiative has conducted dozens of projects which have contributed to the efficiency, effectiveness, and rigor of life cycle approaches on a global scale. This presentation will address those contributions from the viewpoint of meeting critical needs for maintaining and enhancing the quality of the science underpinning life cycle approaches. It will also place those developments in the context of emerging research and practice from academic, government and business organizations, providing a perspective on the significance of the Initiative's contributions to the science of LCA.
Technical work products of the Initiative generally fall into three broad categories - consolidation and cohesion of life cycle inventory and impact methods (particularly with a view towards how those may support social and sustainability assessments), development of practice guidance and support tools for data and databases, and creation or validation of models for various life cycle impact categories. Instances of these developments will be described along with commentary on their consequences for the LCA practitioner community.

LC07-2

Top 10 points about life cycle every government decision maker should know

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The 10 bullets that government officials should remember about Life Cycle Approaches when considering sustainability decisions is a contribution of the UNEP/SETAC Life Cycle Initiative to the discussions for the next UN World Summit for Sustainable Development.
The Initiative has successfully responded to the call from governments for a life cycle economy as stated in the Malmö Declaration and contributed to the development of a 10-year frame work of programs on Sustainable Consumption and Production (SCP).
"To bring science-based life cycle approaches into practice worldwide"is the Mission of the Initiative and 3 objectives were established to achieve it: enhancing the global scope of life cycle data and methodologies through research and innovation; facilitating the use of life cycle approaches worldwide by business, governments and the general public; and expanding capabilities worldwide to apply and to improve life cycle approaches through education and training.
The 10 bullets were disseminated for the first time amongst government representatives during the High-Level CSD Intercessional Meeting on SCP on 2011 as:
- Every product causes environmental impacts in its supply chain, during its use and in its disposal
- To improve and preserve the world, the different impacts of products must be identified and quantified
- Life cycle assessment is the only standardized international tool for identifying and quantifying
impacts of products
- By identifying impacts, they can be understood and managed by companies and governments
- Environmental impacts affect ecosystems in many different ways
- Ultimately, all environmental impacts affect humans
- Companies and the decision of governments must be made based on which impacts are most important and which should be addressed first
- Importance of impacts depends on your perspective
- All life is connected, how those connections are managed is up to you
- When making sustainability decisions, you must consider the entire life cycle including trade-offs
While the first five bullets introduce key concepts the sixth bullet highlights the strong linkage between the environment and human beings. The last four bullets compell the reader to realize the responsibility of his/her decisions. The conclusion of the presentation sheds light on role of the Initiative to further contribute to government and private sectors at a very timely moment when the new mission for the next years of the Initiative is being shaped.

LC07-3

Strategizing capacity development for life cycle management - cases from Vietnam and Malaysia

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The promotion of life cycle management in companies in developing countries has to build upon capacity to perform and interpret life cycle assessments. Drawing on two case studies: one on pangasius aquaculture in Vietnam and the second on palm oil production in Malaysia, the paper identifies - in these two different national contexts - current capacity constraints and future options for strategizing efforts, which target transition towards sustainable production and consumption. Both cases point to the need for capacity to collect valid and reliable data. New life cycle inventories (LCIs) have to be built to reflect real processes in the main sectors of the national economy. While subsidiaries of foreign owned companies take the lead in adopting a life cycle approach in environmental management as a result of corporate policies, the large sector of medium and small scale companies have few or no incentives in their national context at a time when export markets introduce conditionality concerning sustainable production practices. The case studies also show that most examples of LCA practiced primarily seem to be motivated by concerns about the public image of a particular product in the market place. The most significant driver currently seems to occur, when a vital product in the export profile of a developing country is contested on the export markets for its environmental impacts. In conclusion, to move beyond the awareness of life cycle thinking and the communication of 'greener' brands, the linear model of rolling-out and implementing LCA practices in developing countries, which basically is derived from requirements of the LCA methodology itself, the needs revision. Establishing knowledge and data resources, facilitating communication and training, providing limited support for application, and creating international networks for research definitely contributes to capacity development. However, a coherent strategy - drawing on the paradigm shift initiated by UNDP in 2002 and subsequent research on the concept of capacity development - is needed to identify options for interventions for direct stakeholders, for entities in the enabling institutions, for foreign investors, and for regulatory authorities in economic and industrial policies and foreign trade relations.

LC07-4

Water use in life cycle assessment and water footprinting: outputs and prospects of the working group WULCA

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Water use has been largely neglected in LCA of the first decades. While some water use data has been collected in inventories, environmental impacts related to use and consumption of this vital resource have not been addressed until 5 years ago. At this time different research groups have started to develop methods to quantify impacts, and the UNEP-SETAC life cycle initiative has established the working group for water use in life cycle assessment (WULCA).
The group is organized by a core of researchers and practitioners actively contributing to the development of the field, while a larger group is involved in rounds of feedbacks and invited to meetings in order to allow input from various stakeholders in a very vast and dynamic field.
The deliverable of the group was to compile a consistent framework for addressing the environmental impacts related to the various types of water use and areas of protection affected. Another challenge was to establish a common terminology. As a result, the core of the group published a scientific article which builds the basis for future research in this area. In a second phase, the group focused on comparing different available methods, comparing their scientific quality, completeness and applicability on order to provide guidance to LCA practitioners and other interested people about the status of inventory data and impact assessment methods. A scientific paper will be submitted in December 2011.
The working group is also involved in the standardization process of water footprinting, cooperating with research partners and practitioners outside the LCA community in order to contribute to a standard that is compliant with the LCA perspective.
Future action points are the harmonization of existing LCIA methods and inventories. Building up on the methodological review, quantitative comparison of different approaches targeting similar impacts are performed to derive estimates of robustness, while research of missing impact pathways is fostered. Inventory data collection has

been of lower priorities so far, however, with increasing demand for both robust water use information and related impact assessment, the supply of representative water use data it becomes a relevant issue, especially due to the high spatial variability of water use and related impacts.

LC07-5

Value of a Life Cycle approach in evaluating the environmental impacts of packaging for food and beverage applications

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An articulation of the benefits of the life cycle approach to design, manufacturing, use and end of life management of packaging for food applications is important to further examination of the role of packaging within the nexus between security and safety of packaging in food and beverages and environmental protection. Key items of focus for the research and analysis included, but not limited to:
- What is the value of a life cycle approach for beverage and food products and packaging?
- What is the value of including all life cycle stages in evaluating the packaging/food systems to reduce overall life cycle impacts?
- What is the value of including multiple impacts in evaluating the packaging/food systems to reduce overall life cycle impacts?
- What is the value of including the food and/or beverage into an evaluation of the packaging life cycle impacts?
- What characteristics of future LCA studies should be considered when evaluating the food/packaging life cycle?
- Examples of how the waste management hierarchy and LCA results interface/connect

This presentation will present the results of study to examine the Value of a Life Cycle Approach in Evaluating the Environmental Impacts of Packaging for Food and Beverage Applications.

RA01 - Applying models to risk assessments: from the organism to the ecosystem level

RA01-1

How do adverse effects on individual endpoints translate to effects at the population level?

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Toxicity of chemicals is measured on many individual endpoints: feeding, growth, reproduction, and survival. The sensitivity of these endpoints of model species to chemicals is used to gauge the negative effect these chemicals will have on higher levels of biological organization such as populations. However, when using different individual endpoints to estimate risk at the population level, it is important to know the relative sensitivity of populations to changes in different endpoints. For example, is a 20% reduction in feeding more harmful to a population than a 20% reduction in reproduction? In part, these types of questions have been addressed via "elasticity analyses"using matrix models. Using elasticity analysis, the sensitivity of population growth rate to changes in different generalized modes of action (reduction in survival, reproduction, or growth) is calculated. While this provides a useful estimate of relative sensitivity of one important aspect of populations, intrinsic growth rate alone does not define the dynamics of populations. Most population's dynamics are driven in some way via an interaction with their prey species, and a change in the dynamics of individuals may alter this interaction in a way not described by the population growth rate.
We overcome this problem by using a method which considers the interaction of the population and its prey and their dynamics in time by using an individual-based model (IBM). Specifically we use the recently developed framework DEB-IBM (Martin et al. in press). The DEB-IBM framework is an implementation of the Dynamic Energy Budget (DEB) theory in an individual-based modeling context designed to extrapolate from individuals to populations. In this framework DEB provides the rules for how environmental conditions (food, temperature, toxicants) are translated into individual performance (growth, reproduction). DEB theory is generic, as differences between species are described via different parameter values within the same model framework. Using DEB-IBM (http://cream-itn.eu/projects/wp-1/daphnia-2/deb-ibm), we parameterize a model for *Daphnia magna* with individual level data and validate the model under control and exposure conditions at the population level. We then use this to predict the sensitivity of populations to reductions in various measures of individual performance (feeding, maintenance costs, reproduction, and survival) due to hypothetical chemical stressors in dynamic environments.

RA01-2

Exploring the consequences of spatial heterogeneity in pesticide exposure using an individual-based model of collembolan populations

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Suitable habitat for soil organisms may be scarce, thus leading to locally high population densities, because soil, being more static than water or air, is heterogeneous: physical conditions often vary widely on a scale of a few centimetres. Moreover, toxic chemicals are likely to be unevenly distributed in the soil as well. To explore the consequences of these heterogeneities for the population dynamics of soil invertebrates, we developed a spatially explicit individual-based model of the collembolan *Folsomia candida*.
In the model, individuals are assumed to sense and avoid contaminated habitat with a certain probability, which depends on contamination level: avoidance of toxicant influences the feeding behaviour of the organisms, and this in turn affects all the other biological processes. Model rules and parameters are based on data from the literature; for toxicity, only data from standard laboratory tests (survival, reproduction and avoidance) are used. The model has been parameterized and evaluated using Pattern Oriented Modelling (POM): in POM, models are required to simultaneously reproduce a diverse set of patterns.
The model has been run with two simulation scenarios where polluted area and concentrations of toxicant ($CuSO_4$) are the same, but spatial arrangement and connections between clear patches are different. In both cases the presence of patches of suitable habitat allows the population to grow, although the size is reduced with respect to the control. At the lowest concentration, the organisms cannot sense the toxicant and therefore do not avoid the contaminated areas: for this reason toxic effects are much less than proportional to the concentration. From the comparison of the two scenarios, it appears also that when the population is more affected during the spring peak, it is then more resistant during the fall peak, and vice versa.
To conclude, a combination of spatial heterogeneity and stressors can lead to unexpected effects of toxicants at the population level. Individual-based models help disentangle and understand these effects and therefore add ecological realism to environmental risk assessment of chemicals.

RA01-3

A comparison of deterministic and stochastic matrix population models to evaluate ecological risk of chemicals

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Environmental management decisions regarding toxic chemicals are mainly based on measurements on individuals, e.g., mortality and fertility. However, the aim of environmental management is, most often, to protect populations, not individuals. The necessary extrapolation from individuals to populations introduces a large degree of uncertainty in the risk assessment process. Presently, this uncertainty is dealt with by using fixed safety factors that are set to be protective in the majority of the cases. One method to reduce this uncertainty may be to use population models. However, before such models can be used routinely in ecological risk assessment of chemicals, the types of models to use must be determined as well as the level of model complexity necessary to provide an accurate risk assessment for different management scenarios. The objective of the present study was to determine whether simple deterministic matrix population models can be used as a first tier in risk assessment of a chemical, or if more complex models that include environmental stochasticity are needed. Matrix population models for two species of fish (eelpout and perch) were used in combination with dose-response data for a metal mixture, 2,3,7,8-tetrachlorodibenzo-p-dioxin, and tributyltin. From the deterministic models, the maximum acceptable exposure was determined as the level where the population growth rate (λ) is equal to one, which means that the population size is stable. For the stochastic model, the 5th percentile for λ=1 was used, which means that there is 5% probability for population decline. The results were compared to traditional risk ratios, based on individual level responses, and safety factors (in accordance with European Union guidance documents). Although the results of the stochastic models are more informative with regards to probability for adverse ecological effects, the results of the deterministic models clearly reduced uncertainty compared to the traditional risk ratios. This means that simple deterministic models, in combination with appropriate safety factors, can reduce the risk for over- as well as underprotective risk assessments.

RA01-4

Stochastic density dependent matrix model to extrapolate effects of toxicants from laboratory tests to population-level effects: case study on Folsomia candida exposed to cadmium

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Ecological risks of toxic chemicals are usually assessed on the basis of individual responses, such as survival, reproduction or growth. These data could be more effectively exploited if they served to predict effects at higher levels of ecological organization. This can be achieved by means of mathematical and simulation models. When extrapolating from the individual to the population level, environmental stochasticity and other key ecological processes should be taken into account to assure more precise and unbiased results. This study is aimed at developing a general model framework for extrapolating laboratory based individual-level effects of toxicants to populations in the field by considering environmental fluctuations and effects of density-dependence. The practical aplicabiliy of the model was illustrated for a Folsomia candida population exposed to cadmium and influenced by seasonal variation of temperature and density dependence.
The general structure of the model was based on an age-structured Leslie matrix. The effects of fluctuating temperature were linked with vital rates through a series of projection matrices for a range of temperature intervals. Individual-level effects of chemicals were based on classic deterministic dose-response relationships for survival and reproduction. Density dependence function is included in the stochastic matrix model directly by developing a logistic equation analogous to unstructured population model.
The technique outlined here allowed us to include effects of environmental fluctuations and density dependence in matrix population models. This can enhance the capability of matrix models to extrapolate individual-level effects of chemicals to the population level. The developed model is generic and can be adopted for any study with few modifications. The data inputs required for the model are based on the standard OECD test endpoints and annual climate data required for the study area under consideration. In the simulations the population growth rate at constant or mean annual temperatures are always greater than the stochastic population growth rate at the same contamination levels. Our model shows that neglecting density dependence in populations and variability of environmental conditions may seriously underestimate extinction probabilities in toxicant-exposed populations. Whether density dependence aggravates or counterbalances effects of toxicants on populations may depend on whether $\lambda>1$ or $\lambda<1$.

RA01-5
Applying an AQUATOX Aquatic Ecosystem Model with FOCUS exposure scenario to assess pesticide effects
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Aquatic ecosystem modeling can complement empirical approaches to pesticide risk assessment by allowing efficient evaluation of indirect effects mediated through species food-web interactions, testing of multiple exposure scenarios, and assessment of potential long-term effects and recovery times. In a companion poster presentation, we report on the development and calibration of an aquatic ecosystem model based in AQUATOX (version 3.0) for evaluating the potential direct and indirect ecological effects of HerbicideX (hypothetical name) on freshwater systems. We report here on the expansion and application of the calibrated model to: 1) assess potential community-level effects of HerbicideX in a generalized stream characteristic of agricultural areas of northern Europe, 2) demonstrate dose-responsiveness of the AQUATOX stream model, and 3) estimate recovery times of the biological community and key species for cases (if any) where HerbicideX causes significant effects.
The R1 Stream Scenario of FOCUS (2001) was used as the basis for the site characterization and parameterization of physical and chemical elements of the stream model. Nutrient loading similar to HerbicideX experimental mesocosms was used. A fish species (three-spined stickleback) and a dragonfly species (common club-tail) were added to the previously calibrated model, which already had phytoplankton, periphyton, zooplankton, benthic and epiphytic macroinvertebrates, and macrophytes. Immigration and emigration (drift) terms were also parameterized. Information on toxicity and environmental fate of HerbicideX was obtained mainly from the Draft Assessment Report developed by the responsible Rapporteur Member State. An annual time series of exposure concentrations for HerbicideX was developed from a TOXSWA fate model based on the R1 Stream Scenario (i.e., a realistic worst-case scenario). Almost all model species (or groups) showed negligible differences (<3 percent) between control and HerbicideX-exposed cases based on the FOCUS (2001) R1 Stream Scenario, including model species or groups of phytoplankton, macrophyte, zooplankton, benthic/epiphytic invertebrates, and fish. Overall, the behavior of the mesocosm-mimic and generalized stream models follows an expected pattern for aquatic systems, with model species responding to physical-chemical conditions and trophic interactions in ecologically realistic ways.

RA01-6
An ecosystem model for risk assessment of aquatic environments impacted by endocrine disrupters
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Endocrine disruption has been measured in many aquatic environments across the world but the consequences on the whole ecosystem are still unclear. Experimental approaches for characterizing the ecological impact of such disturbances are costly and time-consuming. Therefore, ecological models are currently being developed to support risk assessors in their decisions. Ecosystem models are required for assessing effects at high levels of organization, but the need for extensive calibration for a specific ecosystem limits their application in ecological risk assessment. This study aims at providing risk managers with an ecosystem model able to predict critical changes in aquatic environments impacted by endocrine disrupters. The objective is to find a compromise between the data available and the complexity required for the model. The ecosystem model is developed with field data obtained from a multi-year whole-ecosystem study performed at the Experimental Lake Area (ELA, Ontario, Canada): (i) two years of reference data (ii) three years of exposure to environmentally-relevant concentrations of the synthetic hormone 17α-ethinylestradiol (EE2) and (iii) five years of recovery data. EE2 was chosen because it is one of the most widespread and potent endocrine disrupters. Indeed, the fathead minnow population collapsed after the second year of EE2 additions and endocrine disruption was observed in the other fish species as well. The developed ecosystem model considers direct effects of EE2 on fish species but also the consequences on the whole ecosystem through ecological interactions i.e. feeding and competition relationships. The model is based on simplified equations of the AQUATOX model (USEPA, 2002) with additional equations for endocrine disruption. Three fish classes are used (juveniles, females, and males) with a variable representing the reproductive ability associated with each class. The physical dynamics of the lake (stratification and mixing) was successfully modelled as well as the dynamics of zoo- and phytoplankton naturally present in the experimental lake. This ecosystem model was developed with a focus on EE2-endpoints reliable for risk assessment and will be validated with data from other whole-ecosystem studies performed at the ELA. Further model development will also allow for predicting the percentage of intersex fish, males, and females.

RA02 - Approaches for comparative hazard and risk assessment of chemicals

RA02-1
PRiME - an approach and web-based tool for the comparative risk assessment of pesticides
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Most approaches for the comparative assessment of pesticides are hazard-based. They typically score combinations of fate and toxicity endpoints from standard laboratory tests. Application rates may or may not factor in this comparison. The best approaches derive exposure estimates through models, as regulatory authorities typically do. However, even those approaches that attempt to combine toxicity and exposure into an actual measure of risk, fail in a number of key areas: 1) Adequately addressing inter-species differences in toxicological susceptibility, a key source of uncertainty; 2) Including local conditions such as rainfall, proximity to water bodies and soil type to produce a context-specific risk score; 3) Adjusting risk scores for application methodology; 4) Calibrating the estimated risk score against documented field impacts. The Pesticide Risk Mitigation Engine (PRiME) was designed to address all of these key areas. It was developed with the support of a Conservation Innovation Grant administered by the U.S. Department of Agriculture's National Resource Conservation Service as well as with time and resource contributions from numerous partners in the agricultural and food industry sectors. PRiME uses acute and other toxicity endpoints from both regulatory and non-regulatory tests on a wide range of species. Species-sensitivity distributions are used to derive taxon-specific endpoints. Fate and runoff models are run to assess likely environmental exposures and risk scores are calculated for a number of environmental and human receptors across a selection of pesticides. Most of those scores are estimated probabilities of harm or undesirable effect. Risk is presented on a low /moderate/high scale for final output to the user. Risk score indices designed to date are described. Others (e.g. pollinators) are in development.

RA02-2
An approach for environmental risk assessment of pharmaceuticals by using fuzzy AHP
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Pharmaceuticals in the environment is one of the mostly studied topics for three decades. There are significant amount of studies that are effect directed and do not indicate conclusive results on risks caused by pharmaceuticals. Moreover, everyday new pharmaceuticals are released to markets and it is difficult to predict environmental effects of them. Risk is the combination of likelihood (RL) and probability (RP) of an event and the strenght of the reults (RS) of this event. Fuzzy analytic hierarchy process (FAHP)

provides to organize these criterias systematically and conclude priority numbers for the risk management activities. Risk magnitude (RM) can be inferred by assesssing expert opinions instead of strict formulatios. Fuzzy inference (FI) systems are used for complex matrices that cannot be regulated or formulated. It is aimed to propose an approach for ERA of pharmaceuicals based on FAHP and FI system as an objective and sensitive method in order to overcome uncertainities and compansate data gap in literature. A separate hiererchy was developed for RL, RS and RP in order to get the scores of AHP for inference of RM. Characteristics of the pharmaceuticals and environment under evaluation were conssdered as the subfactors of the RL in order to assess fate/transport of the pharmaceutical in the environment and possible exposure pathways for the ecosystem. Effect assessment is conducted by using RS hierarchy including subfactors of ecotoxicological effects of pharmaceuticals and environmental characteristics that contribute the magnitude of these effects. RP hierarchy contains the sources of the pharmaceuticals and factors related with treatibility indicating the possibility of release to environment. AHP scores of these factors were combined by using fuzzy inference (intersection and union operations) based on expert opinions and RM for the case evaluated is achieved. Risk assessment of pharmaceuticals in the environment by using AHP provide to consider all of the factors contribute to risk both related with pharmaceuticals and environment in terms of risk components that are RL, RS and RP. FI method enables to use expert opinions instead of ampric formulations which is beneficial for the complex assessments that are affected by numerous factors and cannot be completely formulated like ERA. Proposed approach reduces uncertanities and subjectiveness and provides more rigid RM that can be used as a guide for the risk management attributes.

RA02-3

Exposure hazard assessment: lessons learned from cyclic volatile methyl siloxanes

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Two cyclic volatile methyl siloxanes , octamethylcyclotetrasiloxane (D4) and decamethylcyclopentasiloxane (D5), have recently been subjected to close scrutiny of their exposure hazard by the European Union. These chemicals have unusual physical chemical properties which place them outside of the domain of well-studied organic chemicals. It is thus not surprising that difficulties were encountered when existing methodologies for exposure hazard assessment were applied to these chemicals. Here we explore these difficulties with the aim of extracting the lessons that can be learned from these chemicals.
The D4 and D5 cases illustrate nicely that persistence should be assessed for individual media, but they also make it clear that the assessment should be conducted in a multimedia manner for each medium. A further lesson is that it can be necessary to consider differences in the standard of care to be applied to different environments in the context of exposure hazard assessment. Considering bioaccumulation, these chemicals make it clear that the TMF cannot be applied as a gold standard of bioaccumulation assessment to all chemicals. As with persistence assessment, a multimedia perspective in the assessment of bioaccumulation is also useful. Finally, we argue that persistence should have a clear priority over bioaccumulation in exposure hazard assessment.

RA02-4

A new methodology for PBT prioritization of chemical inventories

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A new PBT prioritization methodology has been developed in view of regulatory requirements for quantitative assessment of persistence, bioaccumulation potential and toxicity of chemicals. CATALOGIC/OASIS and EPI Suite QSAR models for calculating P, B and T endpoints have been used. The methodology is implemented in a software system for computerized PBT classification of large chemical inventories.
The developed methodology introduces fate/hazard classification of chemicals based on regulatory thresholds for identifying PBT substances. Thresholds corresponding to the variation of respective test procedure results are further introduced defining uncertainty bright lines around the central threshold values. The model applicability domain of each used QSAR model is incorporated in the scheme in order to evaluate confidence of obtained estimates.
The developed approach introduces a two-stage PBT classification scheme - primary classification of parent chemicals and secondary classification of stable degradants identified by OASIS biodegradation models. Single P, B and T screening results and their associated confidence are used in order to assign parent chemicals to a priority class. The introduced secondary classification based on stable degradants provides an in-depth PBT profile. Following a more conservative approach of applying the prioritization scheme, identification of a hazardous stable degradant is considered grounds for inclusion of the parent chemical in a higher priority class.

RA02-5

Comparative risk assessment of arsenic trioxide and its substitutes for occupational exposure in Murano (Venice, Italy) artistic glass production

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Arsenic trioxide is included in the Candidate List of Substances of Very High Concern (SVHC) and soon it could be subject to authorization under the REACH regulation, because of its properties of carcinogenicity, mutagenicity and toxicity for reproduction (CMR substance). In the district of Murano artistic glass (Venice, Italy), arsenic trioxide has being used since centuries as additive for refining and bleaching melting glass. It is estimated that about 8 tons per year of arsenic trioxide are currently used in Murano glassworks. Small particles of arsenic powder can be easily inhaled by workers; furthermore, when melting the glass mixture at high temperatures, arsenic toxic fumes are released. To reduce the occupational health risks of glass production, the use of suitable substitutes for replacing arsenic trioxide is being explored and cerium oxide and blast furnace slag are among the most promising candidates. A comparative study has been performed with the aim of evaluating the occupational health risks of substitute substances in comparison with arsenic trioxide. Specifically, the objectives of this study are: i. to assess arsenic trioxide health hazard in comparison with cerium oxide and blast furnace slag; ii. to develop for all production phases suitable exposure scenarios for workers, representative of a typical glassworks; iii. to quantify inhalation and dermal contact exposure to arsenic trioxide and its substitutes through the application of different occupational exposure models (i.e., ECETOC worker tool, MEASE and ART) and to compare models' performance for inorganic substances in the selected exposure scenarios; iv. to estimate and compare health risks for glass workers associated to inhalation and dermal contact for the substances of interest. The comparative risk assessment procedure proves to be effective in demonstrating that the use of cerium oxide and blast furnace slag would reduce the health risks associated to occupational exposure. Cerium oxide and blast furnace slag are therefore confirmed as interesting candidates to replace arsenic trioxide in artistic glass production.

RA02-6

Comparative hazard and risk assessment of flame retardants (Prototypical Case Study): ENFIRO

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Several brominated flame retardants (BFRs) have unintended negative effects on the environment and human health. Some of them show a strong bioaccumulation in aquatic and terrestrial food chains, some are very persistent, and some show serious toxicological effects such as endocrine disruption. During the last decade, an increasing number of reports have presented evidence of these negative effects caused by BFRs. A number of BFRs (in particular polybrominated diphenyl ethers (PBDE's), hexabromocyclododecane (HBCD) and tetrabromobisphenol-A (TBBP-A)) can be found in increasing concentrations in the human food chain, human tissues and breast milk [1-4]. Less toxic alternatives appear to be available already but comprehensive information on their possible toxicological effects are lacking. The European Commission-funded project ENFIRO investigates a prototypical case study on substitution options for some BFRs and compares the hazard, risk, fire performance and application of the alternatives versus the BFRs. In addition, a comparative life cycle assessment is carried out. The current paper address the ENFIRO approach, and discuss and explore different comparative (hazard) assessment approaches for halogen free flame retardants (HFFRs) and BFRs, as guidance documents are still lacking on comparative assessments. In conclusion, the US EPA and Green Screen PBT thresholds were more suitable in comparative hazard assessments due to larger number of threshold categories compared to REACH. The challenge in a substitution study is not only to perform a comparative hazard and risk assessment, but also to integrate additional highly important factors, in the case of flame retardants these are fire performance, technical application, life cycle, and costing aspects. The use of decision support systems for this integration was explored.

RA03 - Are Environmental Specimen Banks ready to face future challenges of environmental chemistry and regulatory toxicology?

RA03-1

A fish tissue archive for monitoring chemical pollution in UK rivers. How it operates and its application to EU priority substances

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The UK Fish Tissue Archive

In 2007 CEH and the Environment Agency in England and Wales (EA) began to build a fish tissue archive by collecting 10 fish (generally roach) per year from a number of river sites and storing them long term at -80°C to provide a resource for future retrospective monitoring of pollutants.
Measuring pollutants in biota is often preferable to water because fish and other biota accumulate chemicals both from the water and the food chain over their lifetime,

making the values less variable, more relevant to the potential threat to flora or fauna, or easier to measure because the concentrations are higher.
Environmental Quality Standards (EQS)
EU Directive 2008/105/EC lists freshwater EQS for over 30 substances, but it only includes an (optional) biota standard for 3 (article 3, 2a) requiring member states that use this option to "apply, for mercury and its compounds, an EQS of 20 µg/kg, and/or for hexachlorobenzene, an EQS of 10 µg/kg, and/or for hexachlorobutadiene, an EQS of 55 µg/kg, these EQS being for prey tissue (wet weight), choosing the most appropriate indicator from among fish, molluscs, crustaceans and other biota"
Results
We analysed some of the fish from the UK Fish Tissue Archive for these three substances and found:
Mercury, which was used in many industrial and agricultural applications in the past and is still released as a trace component of fossil fuels and some electrical components was analysed in roach. About half the samples exceeded the EU EQS of 20 µg/kg (median: 23 µg/kg), but even the maximum of 68 µg/kg is about a factor of 10 below the EU food limit of 500 or 1000 µg/kg depending on fish species.
Hexachlorobenzene, a fungicide which is no longer used in the EU, was below the EQS of 10 µg/kg in all fish analysed. Eels had higher concentrations with a median of 1.8 and a maximum of 6.4 µg/kg compared to 0.9 and 4.5 µg/kg in roach.
Hexachlorobutadiene which was in the past used as a solvent in polymer production and as a fungicide and seed dressing and is still generated in small amounts as a by-product, was not detectable in the majority of samples.
Conclusions
- The samples stored in the Fish Tissue Archive are well suited for monitoring of priority substances, especially those for which an EQS has already been set.
- Mercury levels are of some concern in English rivers.
- As the Fish Archive grows it will become possible to determine temporal and spatial trends of these and other substances

RA03-2
Environmental monitoring data: support for an effectiveness assessment and a success control under REACH
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Environmental specimen banks support competent authorities in the assessment of chemicals. Together with national and EU-wide monitoring systems they can give information for the identification of new substances of regulatory concern. Beyond the assessment of individual chemicals, monitoring data can also be used to develop indicators to evaluate the implementation of different chemical regulations by providing information on the impact of chemicals to human health and different compartiments of the environment.
By June 2012, the European Commission has to present a first evaluation of the effectiveness of the REACH regulation. Human biomonitoring and environmental monitoring programmes may provide valuable data to underpin this evaluation. In the EU there is a variety of environmental monitoring activities which have been established for various reasons. They are - in different degrees - suitable to indicate the implementation of REACH. A research project - funded by the German Environment Protection Agency (UBA) - analyzed the available monitoring programs (including environmental specimen banks) to identify those who can contribute to evaluate the effectiveness and success of different REACH task, starting from specific tasks related to specific parts of REACH (e.g. registration) up to tasks related to the effectiveness evaluation of REACH as a whole.
In order to determine appropriate indicators and methods to evaluate the impact of the European chemicals legislation REACH, a detailed and complete review on ongoing environmental moni¬toring activitieshas been conducted. Furthermore, a guidance document for the use of environmental monitoring data with a view to the evaluation of chemicals has been developed and presented. It includes both the company's self-monitoring as well as government monitoring and important regulatory focal points under REACH. Exemplary case sheets on selected chemicals were documented for the monitoring / identification of substances of concern, thereby using the Environmental Specimen Bank (ESB).
Future challenges in regulatory risk assessment go beyond time trends of individual substances. Effectiveness assessments of regulations such as REACH require indicators for the total environmental burden due to the wide dispersive uses of a large number of substances - and its effect on biodiversity. Environmental specimen banks can support such assessments and the elaboration of adequate indicators.

RA03-3
Mercury stable isotopes in seabird eggs from the NIST Marine Environmental Specimen Bank reflect a gradient from terrestrial geogenic to oceanic mercury reservoirs
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The Seabird Tissue Archival and Monitoring Project (STAMP) is a collaborative effort run by the U.S. Fish and Wildlife Service Alaska Maritime National Wildlife Refuge (USFWS-AMNWR) and the National Institute of Standards and Technology (NIST) as a systematic, long-term program to monitor persistent organic pollutants (POPs), mercury, and other contaminants in Alaska's marine environments using seabird eggs. Eggs are collected and processed using established protocols and shipped to NIST's Marine Environmental Specimen Bank (MESB) at the Hollings Marine Laboratory in Charleston, South Carolina, for long-term (decadal) cryogenic storage. To date, over 1600 clutches of eggs have been collected across 1000's of kilometers of Alaska's marine environment. This systematic and broad scale effort has provided a valuable archive of samples to select from for environmental contaminant research. Elevated mercury concentrations ([Hg]) were found in Alaskan murre (Uria spp.) eggs from the coastal embayment of Norton Sound relative to insular colonies in the northern Bering Sea-Bering Strait region. Stable isotopes of Hg, carbon (C), and nitrogen (N) were measured in the eggs to investigate the source of this enrichment. Lower δ13C values in Norton Sound eggs (-23.3 to -20.0 ") relative to eggs from offshore colonies (-20.9 to -18.7 ") indicated that a significant terrestrial C source was associated with the elevated [Hg] in Norton Sound, implicating the Yukon River and smaller Seward Peninsula watersheds as the likely Hg source. The increasing [Hg] gradient extending inshore was accompanied by strong decreasing gradients of δ202Hg and Δ199Hg in eggs, indicating lower degrees of mass dependent (MDF) and mass independent Hg fractionation (MIF) (respectively) in the Norton Sound food web. Negative or zero MDF and MIF signatures are typical of geological Hg sources, which suggests murre in Norton Sound integrated Hg from a more recent geological origin that has experienced a relatively limited extent of aquatic fractionation relative to more oceanic colonies. The association of low δ202Hg and Δ199Hg with elevated [Hg] and terrestrial δ13C values suggested that Hg stable isotopes in murre eggs effectively differentiated terrestrial/geogenic Hg sources from oceanic reservoirs.

RA03-4
Temporal trends in dioxins and dl-PCBs from Baltic herring (Clupea harengus)
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The unintentional release of dioxins (dibenzo-p-dioxin (PCDD), dibenzofuran (PCDF), and dioxin like PCBs (dl-PCB)) into the environment was at its peak prior to the 1980s [1]. Since then, extensive measures have been taken to reduce dioxin emissions within the EU e.g., the Helsinki Convention (1974, 1992), the Stockholm Convention on Persistent Organic Pollutants (POPs), the plan for integrated pollution prevention and control (IPPC) [3]. However, dioxin concentrations continue to be higher than expected in Baltic fatty fish. A large proportion of fish caught in the Baltic Sea exceed the limit for marketing fish within the EU [1] (4 pg WHO05-TEQ/g ww (ΣPCDDs+PCDFs); 8 pg WHO05-TEQ g/ww (ΣPCDDs+PCDFs+dlPCBs)) [2] and thus, ongoing environmental monitoring occurs in many Baltic countries.
Within the Swedish National Monitoring Programme, Baltic herring, Clupea harengus, a fatty fish consumed by humans, are analysed yearly for dioxin concentrations. As dioxins are lipophilic, fatty fish tend to bioaccumulate greater concentrations of these contaminants compared to lean fish species. Here, yearly monitoring data of herring from three sites on the east and one site on the west coast of Sweden are presented. The aim of this work is to monitor and detect temporal trends and changes in dioxin concentrations over time in a fish species of importance for human consumption and top marine predators. Results are used to inform policy and regulation makers so dioxin guidelines can be adjusted accordingly.

RA03-5
Temporal trends in human exposure to fluorosurfactants and related chemicals in two cities from Germany
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A total of 420 samples collected from the period of 1981-2009 and from two cities in Germany: Münster (n = 10 samples (5 male and 5 female) per year from 1981-2009 (no sample for 1994), for a total of 270 samples) and Halle (n = 10 samples (5 male and 5 female) per year from 1995-2009, for a total of 150 samples), were analyzed for a suite of fluorinated analytes. The specific targets include current and legacy commercial fluorinated surfactants, such as the polyfluoroalkyl phosphoric acid diesters (diPAPs), the N-ethylperfluorooctanesulfonamidoethanol-based polyfluoroalkyl phosphoric acid diester (SAmPAP), and the perfluoroalkyl acids (PFAAs). Both the diPAPs and various PFAAs, that include PFOA and PFOS, have been detected in human blood., Among the 420 samples analyzed here, the perfluorosulfonates (PFSAs: i.e., C6 (0.053 - 3.83 ng/g)

and C8 (0.318 - 79.0 ng/g)), perfluorooctanesulfonamidoacetates (N-MeFOSAA (<0.0031 - 8.11 ng/g), N-EtFOSAA (0.0058 - 9.00 ng/g), FOSAA (<0.0011 - 8.25 ng/g)), and the perfluorocarboxylates (PFCAs: i.e., C8 (0.176 - 31.7 ng/g), C9 (0.020 - 2.70 ng/g), C10 (0.020 - 0.880 ng/g), C11 (0.003 - 0.555 ng/g) were detected in over 80% of the samples. The long-chain PFCAs (C12 (<0.0017 - 0.056 ng/g) and C14 (<0.0017 - 0.049 ng/g) PFCAs), however, were only detected in 20% of the samples. Temporal trends can be observed for some of the analytes: PFOS concentrations peaked in 1986 (~ 30 ng/g) and reached a plateau before they began to decrease starting in the year 2000 until 2009 (~ 4 ng/g) in Münster samples. A similar decline in PFOS concentrations (1995-2009) was also observed for samples from Halle. The temporal trend observed here for human PFOS contamination mirrors industrial production patterns, with the post-2000 decline in PFOS sera concentrations occurring concurrently with the phase-out of PFOS and related chemicals starting in 2000. A total of 320 samples were analyzed for DiPAPs and SAmPAP, although quantifications had been done only for 6:2/6:2 and 8:2/8:2 DiPAPs due to the limited availability of analytical standards. Further confirmation using matrix matched calibration curve and standard addition will be carried out for 4:2/4:2, 10:2/10:2, and SAmPAPs. The 6:2/6:2 (<0.00048 - 0.762 ng/g) and 8:2/8:2 (<0.0004 - 0.285 ng/g) diPAPs were detected in 46% and 32% of the samples, respectively. No distinct was observed for 8:2/8:2 DiPAP, however, an increasing trend could be observed for 6:2/6:2 DiPAP after year 2000.

RA03-6

New challenges for environmental specimen bank applications - banking for marine mammal health research

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For 33 years the National Institute of Standards and Technology (NIST) has been banking environmental and biological specimens emphasizing long-term storage under cryogenic conditions to minimize sample degradation over time, use of special materials and procedures for specimen collection and handling, to minimize the possibility of introducing an artifact into the sample and thus biasing the analytical results, and well documented and published standard protocols and procedures covering all steps in sampling and banking including collection procedures, sample handling and processing, specimen transport, bank specimen log-in and tracking procedures, and continuous recording of specimen storage conditions over time. Presently, the banking program of NIST is centered at its Marine Environmental Specimen Bank (Marine ESB) that is located at the Hollings Marine Laboratory, Charleston, South Carolina, USA. The greatest number of specimens in this bank with the widest geographic coverage is marine mammal tissues. These tissues are collected and banked primarily for retrospective studies of contaminants in these aquatic animals. The banking of marine mammal tissues began in 1992 as part of the National Oceanic and Atmospheric Administration's (NOAA's) Marine Mammal Health and Stranding Response Program (MMHSRP). In 2003, NIST began collaborating with organizations and researchers on the U.S. east coast in studies to assess the health of bottlenose dolphins, Tursiops truncates. This health assessment and banking approach is being expanded to other marine mammal species and to other regions of the US. Based on the experience gained through the bottlenose dolphin health assessment project and an ongoing marine mammal studies related to the recent Gulf of Mexico oil spill incident, NIST is working with NOAA and its collaborating partners to establish the marine mammal specimen bank as a major resource of samples for integrative animal health research. This expansion will be emphasizing the banking of specimens for wildlife disease studies, determining exposure to biotoxins, and developing health biomarkers, in addition to determining contaminant exposures. This expansion is requiring additional banking expertise, identification of additional kinds of matrices to bank, and the storage conditions required for long-term banking. These and other aspects of the expansion will be discussed.

RA04 - Established and emerging footprints - striving towards a valid and comprehensive support for decision-making processes

RA04A-1

Midpoint and endpoint indicators for global scale terrestrial acidification: a dilemma for decision-making

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For some impact categories, such as climate change, the link between midpoint and endpoint indicators is based on a proportionality factor, which adds relevance, but does not add further discrimination between emitted pollutants. However, for other impact categories, such as acidification, all three modeling steps: fate, sensitivity and effect, add discrimination between chemicals in addition to relevance. Whether to make a decision based on a midpoint or endpoint indicator is an old debate. This paper aims at contributing to this discussion by showing for the first time, the lack of correlation between midpoint and endpoint indicators for acidification, and in light of these results, further discuss the relevance of using midpoint and/or endpoint indicators and the implication for decision makers. Midpoint CFs [(mol [GREEKX] L^{-1}) [GREEKX] ha [GREEKX] (kg S or Nemitted)$^{-1}$ [GREEKX] yr] results from the multiplication and subsequent summation of an atmospheric fate factor (FF) and a soil sensitivity factor (SF). Endpoint CFs [ha [GREEKX] (kg S or Nemitted-1) [GREEKX] yr] were obtained by adding a biome specific vegetation effect factor (EF) to the midpoint CF. CFs were obtained at a worldwide 2°x2.5° (latitude x longitude). FF [(kg S or Ndeposited) [GREEKX] yr^{-1} [GREEKX] (kg S or Nemitted^{-1}) [GREEKX] yr] describes the atmospheric impact pathway from the emission location i of pollutant p to the corresponding deposition in the receiving soil j. SF [(mol [GREEKX] L^{-1}) [GREEKX] (kg S or Ndeposited)$^{-1}$ [GREEKX] yr [GREEKX] ha] translates the change in soil pH according to a change in emission. Changes in the vegetation EF [(mol [GREEKX] L^{-1})$^{-1}$] is a function of biome specific coefficients. The midpoint CF quantifies the concentration of H+ ions (evaluated through pH) and assumes that any change in pH will have consequences on the receiving environment while the endpoint CF evaluates the decrease in species richness of the biome vegetation related to this change in pH. Comparison of results between the midpoint and the endpoint assessment showed the importance of introducing a further modelling step to highlight biomes having vegetation with lower resistance to pH change. They also showed a medium-low correlation (R2 = 0.60) between midpoint and endpoint indicators. This work thus raises questions about which indicator is more relevant for terrestrial acidification and/or should be used since a further modelling step from midpoint to endpoint is no longer synonym of proportionality between the elementary flows and thus LCA conclusions can be inverted.

RA04A-2

Global life cycle impact assessment on marine eutrophication

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As part of the ongoing EU FP7 project LC-Impact (www.lc-impact.eu) new life cycle impact assessment (LCIA) methods are going to be developed and tested on industry cases. Among the life cycle assessment (LCA) impact categories in focus are aquatic eutrophication. As related to especially the marine environment very few and restricted attempts have yet been done on trying to include eutrophication in LCA. The aim of LC-Impact is to develop both a global and a spatial (and temporal) differentiated model, as both central fate processes, sensitivities of receiving environments (e.g. differences in limiting nutrient and variations in this over the year) and the resulting damage can show important spatial variations. Both midpoint and endpoint (damage) modeling are to be included and the aim is to base the damage modeling on dose-response curves expressing the correlation between the (increase in) nutrient concentration and the potentially affected fraction of species in the marine ecosystem. This paper presents the first draft on the midpoint model for global marine eutrophication due to nitrogen emissions for the emission sources "fertilizer in agriculture", "manure in agriculture", "N-fixation in agriculture", "air emissions of NH3", air emissions of NOx and "water emissions"including direct sewage water emissions and emissions after sewage treatment.

RA04A-3

Life-cycle Assessment of biofuels for transportation: understanding the effects of scale

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Several types of biofuels are being used around the world, with typically different biomass feedstocks and pathways of production. Biofuels substitute for gasoline or diesel in transportation. The largest scale conversion of biomass into biofuel is currently taking place in the United States, supplying about 7% of the fuel market by volume. Corn ethanol carries a number of environmental problems. Instead, alternative biomass feedstocks are being considered at a scale not seen ever before. We quantify the effects of scale on the production and use of ethanol. In contrast to the majority of extant research, which focuses on a unit of transportation biofuel but ignores the economic, industrial, and environmental feasibility of delivering billions of units to the final customers, we address the availability of land, the needed agricultural practices, refining operations, and storage and distribution of biofuels at industrial scale. We also study the environmental and human health effects of combusting ethanol in vehicles on large scale. We summarize the experiences and environmental effects of large-scale biofuel production and use in Europe and Brazil, and contrast them to the proposed 40 billion liter biofuel federal mandate by the year 2020 in the United States, partially to be met by conversion of cellulosic matter into ethanol. The crops of choice will be grasses, Miscanthus x giganteus and switchgrass, and crop residues such as corn stover. Life-cycle assessment is used as the framework to study the effects of scale throughout the entire life-cycle of biofuels. Preliminary results indicate that growing biomass for fuel at an industrial scale presents a number of unique challenges as well as opportunities. We show that economies of scale make a decisive difference between industrial-scale and lower-scale ("boutique") biofuels. For the United States, we show that making 40 billion liters of biofuels by a deadline only 9 years away requires careful environmental, technical, and economic planning. We present scenarios for land conversion, trying to answer the question where and on what kind of land will biomass of this scale be grown. We quantify soil organic carbon emissions from massive biomass cultivation, and the need of crops for water, fertilizer and biocides. We assess the greenhouse gas, water consumption, and criteria air emissions of converting cellulosic biomass into ethanol at industrial scale.

RA04A-4

Accounting for greenhouse-gas emissions in LCA from the degradation of chemicals in the environment

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Chemicals are often released into to the environment at their end of life. As they degrade, emissions of CO2 and other greenhouse gases (GHG) occur, which are often excluded from LCA studies. This work addresses this methodological gap by presenting a method to account for (GHG) emissions from degradation, namely carbon dioxide (CO2), methane (CH4) and nitrous oxide (N2O). In addition, carbon accounting rules for biogenic and fossil carbon are discussed and several options are presented that provide a consistent framework for LCA studies.

A Level III fugacity model is proposed to estimate the multimedia distribution and degradation of chemicals released to the environment. The environmental distribution, along with emission factors and assumptions for each compartment (air, water, soil, sediments) is used to calculate emissions of CO2, CH4 and N2O following initial release of the chemical to either the air, water or soil compartments. The method is described and applied to nine organic chemicals. GHG emissions representing the end-of-life stage of these nine chemicals are shown to be significant when compared with the corresponding cradle-to-gate emissions, particularly for those situations where there is no prior waste treatment phase, such as in a wastewater treatment plant. Chemical composition is shown to be important and for three of the nine chemicals and release scenarios the degradation emissions exceeded the cradle to gate phase. For chemicals released directly to water, the total GHG emissions are comparable to those expected if the chemicals are treated in a wastewater treatment plant, including the emissions from energy use of the latter.

In terms of carbon accounting, we show the need to account for biogenic carbon sequestration if a chemical does not degrade at its end of life, as well as the need to correct the Global Warming Potential (GWP) of methane, depending on whether it is of biogenic or fossil origin.

In conclusion, the method presented enables the accounting of GHG emissions that are currently neglected in many LCA and carbon footprint studies. The model has been parameterized for a generic environmental scenario but it can be adapted for more site specific conditions. The main limitation and source of uncertainty is the potential lack of chemical-specific data required to model environmental fate of a chemical. Also, the method uses generic assumptions and emission factors, that might not be appropriate to describe local conditions.

RA04A-5

Water footprint and life cycle assessment frameworks: synergies and hurdles

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Water footprinting has come a long way in the past 10 years, from simple water volume inventories, to scarcity assessment, to damage oriented LCIA modelling of several impact pathways up to endoints. With this increase of methodological developments and applications, the scientific and industrial communities are now debating about the ultimate meaning(s) of a water footprint. This paper aims to evaluate the synergies and hurdles between the so far developed water footprint approaches, with the traditional LCIA midpoint-endpoint framework. We therefore propose to demystify: a) Standalone versus full life cycle assessment water footprint; b) Single indicator versus multiple indicators; c) Midpoint versus endpoint assessment; d) Impacts of water use versus impacts on the water resource and e) Availability of water resource versus water pollution. This discussion is illustrated with a simplified example of aluminium production, where available methods are compared and synergies and contradictions are presented.

The review by Kounina et al. identified several methods for impact assessment in each of the areas of protection: human health, ecosystems and resources. However, these solely assess the potential impacts related to water availability (impacts from water use). Potential impacts from pollution of the resource water (impacts on the water resource) are considered by the traditional LCIA models of, for example, aquatic ecotoxicity, eutrophisation, etc. These two distinct concepts can however lead to common endpoints and we propose to group them into three aggregation level: I) a Water Availability Footprint (WAF), a standalone method which address availability issues from water use, including lowered availability from pollution (but no other impact related to water pollution), II) a Water Footprint Assessment (WFA) as standalone, which includes all impacts of an activity on the water resource or III) as part of an LCA methodology.

The results of the three aggregation levels applied to the aluminium illustrative example show that the WFA profile is fully compatible to the more comprehensive LCA profile, the impact on water resource being a fraction of each LCIA damages on human health, ecosystem quality and resources. The WFA profile, can be further disaggregated putting in perspective the relative contribution of each impact pathway to the overall impacts on the water resource within each area of protection.

RA04A-6

Chemical footprint from point sources in Sweden

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This study has identified a method to quantify the chemical footprint from point sources with data from the E-PRTR (European Pollutant Release and Transfer Register) togheter with USEtox. USEtox is often used in Life Cycle Impact Assessment.

There is an EU regulation since a few years saying that industrial facilities (e.g. industries) emitting over certain thesholds have to report to a register, E-PRTR, annually. The industrial facilities covers 65 economic activities within the following 9 industrial sectors: energy, production and processing of metals, mineral industry, chemical industry, waste and waste water management, paper and wood production and processing, intensive livestock production and aquaculture, animal and vegetable products from the food and beverage sector, and other activities. Data is provided in the register for 91 pollutants falling under the following 7 groups: greenhouse gases, other gases, heavy metals, pesticides, chlorinated organic substances, other organic substances and inorganic substances. Data was collected from the EEA website, where all E-PRTR data is available for all EU27 countries. The emissions were listed by amount to water and air respectively.

A calculation on the impact is made using the USEtox method as implemented in SimaPro. The USEtox model is an environmental model for characterization of human and ecotoxic impacts in Life Cycle Impact Assessment and for comparative assessment and ranking of chemicals according to their inherent hazard characteristics. In this study the impacts human toxicity (cancer and non-cancer) and ecotoxicity are included. The calculations are performed in SimaPro. The results are given in CTU (comparative toxic units).

The results are for the year 2008. Sweden has delivered emissions for 53 substances, some to air or water and some to both. The total emission to air is very much larger than the total emission to water.The expected results are: an aggregated measure of the toxicity from the sources included in E-PRTR, a calculation on contribution to toxicity by different industry sectors, information on each substance's contribution to toxicity, identification of the most important substances. For these four the results are divided in contribution to human toxicity and to ecotoxicity. This study makes it possible to discuss how useful this method is to quantify the chemical footprint by using data from E-PRTR and the USEtox method.

RA04B-1

Probabilistic environmental hazard assessment of implementing green chemistry property design guidelines to reduce acute and chronic aquatic toxicity

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One of the Twelve Principles of Green Chemistry emphasizes the need to synthesize safer chemicals. These chemicals should be capable of performing their desired function but would be designed to elicit minimal toxicity. In support of this effort, two recent studies by Voutchova et al have explored the relationships between chemical properties and acute or chronic toxicity as measured through standardized OECD and EPA protocols. Mechanistically-rationalized guidelines were derived resulting in two practical design guidlines: acute and chronic toxicity could be minimized if compounds had an octanol-water partition coefficient (log Pow) below 2 and HOMO-LUMO gap (dE) greater than 9 eV. In this study, we examined the potential utility and effectiveness of these design guidelines to reduce acute and chronic aquatic toxicity of common industrial chemicals using probabilistic environmental hazard assessment (PEHA). Chemical Toxicity Distributions (CTDs), a type of PEHA modelling approach, are ideal for predicting the probability of encountering compounds or toxicological thresholds when information is lacking for new chemicals. CTDs were performed: 1. to predict the likelihood of encountering industrial chemicals exceeding established US EPA thresholds of standardized acute and chronic toxicity to algae, cladoceran and fish models; 2. to predict the likelihood of exceeding these thresholds if chemical safety guidelines were followed; and 3. to examine acute and chronically toxic chemicals, chemical classes and modes of action of chemicals that may not be "designed out"by chemical property guidelines. For example, in the absence of chemical design guidelines, our model predicts that 14.5% of chemicals would be classified by the EPA as being of "High Level of Concern"for acute toxicity (LC50 of 0-1 mg/L) to the fathead minnow. However, if log Pow and dE guidelines were employed during chemical development, only 3.3% of industrial chemicals are predicted to be of High acute toxicity concern to the fathead minnow. If the two green chemistry design guidelines put forth by Voutchkova et al are employed, the present study predicts that reduced acute toxicity to the fathead minnow could be achieved for over 10% for industrial chemicals classified with High acute toxicity.

RA04B-2

Biodiversity footprinting - quo vadis?

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Biodiversity loss, and its potential impacts on human welfare, are an increasing environmental concern, and should be assessed in product assessments, in order to provide

adequate support to decision-makers. Likewise, there is an upcoming trend to quantify environmental impacts of products in terms of so-called footprints, which should address biodiversity effects in addition to the conventional carbon and water footprints. However, biodiversity is a multifaceted concept with strong variation in time and space, which makes it difficult to assess. Some current methods are based on the unit "potentially disappeared fraction of species"(PDF), but the scale (e.g. biodiversity loss at the local, regional or global level) and choice of which species should be protected are not consistently defined across impact categories. Therefore, impacts to biodiversity at local, regional or global scales are often aggregated, leading to misinterpretations of LCA results. Here, we attempt to provide a framework to guide methodological choice. Clarifying why we are concerned about biodiversity loss is the first step towards determining what we should be measuring. We distinguish between valuing biodiversity due to intrinsic value or due to its utility for mankind. For the first, enough primary habitat needs to be conserved and the human-modified landscapes need to be managed to avoid global extinction of species. The utility can be manifold and the concept of ecosystem services could serve as a starting point that helps to structure, classify, and measure different functions that ecosystems provide for humans. We also highlight value judgments involved in assessment frameworks, indicators and weighing schemes. To assess cause-effect chains of biodiversity loss, multivariate models, meta-analysis of literature of cause-effects from field surveys, extrapolation of lab experiments or expert opinion can be used.

RA04B-3

Valuating ecosystem goods and services in LCIA

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In LCIA models, resource assessment is centred on the notion of scarcity: depletion is evaluated using a static perspective by comparing a resource's rate of abstraction versus the available stock and its rate of regeneration, or by quantifying the marginal extraction cost. As a result, a limited number of resources (essentially fossil fuels and minerals) is included: ecosystem goods and services (EGS) are basically ignored, despite their crucial role. Dynamic accounting is a prerequisite to consistently embrace the actual pressure of human activity on renewable resources, their marginal rate of regeneration and the interdependence of their production patterns. Hence, ecological modelling can be a way to build a consistent and practical framework of characterization of EGS in LCA. The GUMBO model details the internal behaviour of the global natural system (geobiosphere) and its interactions with the anthroposphere; it is adjusted with key metrics measured during the 20th century to reflect global dynamics. The model delivers the economic values of human, social, built and natural capitals (i.e. EGS) according to user-defined scenarios for the societal mankind during the 21st century. The use of monetary units enables direct comparisons among 'capitals' and is a strong vector to communicating results. However, it drives to a utilitarian, end-user perception of EGS' usefulness, disregarding the role of indirect EGS and the past natural 'investment' to this capital. Therefore, other metrics developed in the field of sustainability indicators may be tested, such as emergy. Acknowledged to be fruitful EGS accounting in LCA, the emergy method provides a measure of the global-scale geobiosphere work with a common physical numeraire (equivalent joules of solar energy, seJ). We expect GUMBO to improve consistency in the emergy evaluation of global natural processes and resulting Unit Emergy Values (UEV) of EGSs, which can be used to obtain complementary (physical) information to the (economic) characterization of EGSs in LCA. Although regionalization of this framework remains unclear, it is expected to be highly representative at global scale and open the road to a comprehensive, ecology-oriented perspective in the evaluation of the natural capital and its use by human systems. The aim of this presentation is to illustrate the methodological approach and its preliminary outcomes.

RA04B-4

Exergetic footprint as indicator to assess the environmental sustainability of processes

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Exergy analysis has two key attributes for being used as an environmental indicator: first, given that the environment is used as a reference state, exergy is a measure of any thermodynamic deviation with respect to its normal state; second, it allows comparisons between inflows and outflows, regardless they are mass or energy streams, using the same physical units (exergy) for their analysis.
Besides, the exergetic footprint (ExF) bears in mind the exergy that still remains in products and highlights the use of exergy as a convenient unit of measure and comparison. In this paper, the (ExF) was used as a resource/waste accounting indicator for the environmental assessment of a production process. The proposed methodology was applied to a wood-based particleboard production process from a factory located in Galicia (NW Spain).
The study was proposed as a gate to gate analysis. The incoming streams were categorised as raw materials, secondary materials and energy sources, while the output streams were the generated waste and the produced particleboard. 1 m3 of produced particleboard was selected as functional unit. Raw material for the production process was wood from pine (75%), black poplar (10%), mixed wood (5%) and recycled wood waste (10%). Additionally, with the aim of assessing the influence of the use of recycled wood as raw material on the ExF, some scenarios of the production process were built considering and increasing ratio of recycled wood used until the complete substitution of the roundwood.
The total exergy consumption for the particleboard manufacturing process was determined as the sum of each input category exergy plus the exergy content of wastes, reaching a value of 17.56 GJ per functional unit. Meanwhile, to determine the ExF the exergy that still remains in the produced particleboard was also considered, and a value of 3.5 GJ per functional unit was obtained. For the scenarios built, CEx ranged from 17.76 to 15.73 GJ·m-3 particleboard and the ExF from 3.69 to 1.66 GJ · m-3, for 0 to 100% of recycled wood wastes employed.
The material resources, especially wood material, were the main contributors to CEx and ExF, as it had been identified by the ecological footprint in a previous work. The results suggest that a clear improvement in the sustainability of the process could be attained by increasing the feasibility of using different waste materials in the design of the particleboard.

RA04B-5

Thermodynamic resource indicators and footprint in LCA: a case study of titania in China

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LCA has standardized methods for assessing emission impacts but no comparable methods for the accounting or impact assessment of resource use. This study contributes to the existing research by offering a comprehensive comparison of different resource indicators, in particular those based on thermodynamics, and testing them in a case study of titania in China.
The system boundary for resource indicators and the case study is defined as a thermodynamic hierarchy at four levels. Seven resource indicators are applied. Four are thermodynamics based: cumulative energy demand (CED), solar energy demand (SED), cumulative exergy demand (CExD), and cumulative exergy extraction from the natural environment (CEENE), and three have different backgrounds: abiotic resource depletion potential (ADP), environmental priority strategies (EPS), and eco-indicator 99 (EI99). The foreground Inventory data has been collected through on-site interviews and visits. The background inventory data are from the database ecoinvent v2.2. Characterizations factors are based on CML-IA database. Computations are with the CMLCA software.
Results show that the scores of resource indicators of the chloride route for titania system are lower than that of the sulphate route except in terms of SED. Within the four thermodynamic indicators for resources, CED, CExD, and CEENE have similar scores while their scores are five orders of magnitudes lower than the SED score. Atmospheric resources do not contribute to the SED or CEEND score. Land resources account for a negligible percentage to the SED score and a small percentage to the CEENE score. Non-renewable resources have a dominant contribution to all seven resource indicators. The global production of titania would account for 0.12% and 0.14% of the total anthropogenic non-renewable resource demand in terms of energy and exergy, respectively. The entropy footprint of global titania is 5.2 E+07 m2.
We demonstrate the feasibility of thermodynamic resource indicators and recommend CEENE as the most appropriate one for accounting and characterizing resource use. As for the three non-thermodynamic resource indicators, they take the different resource issue as their key problem and have higher environmental relevance in terms of expressing the resource scarcity and depletion than the thermodynamic ones. As the conceptual basis for the several indicators differs fundamentally, different cases might well show more diverging outcomes.

RA04B-6

European guidelines for measuring the environmental footprint of products and organisations

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In close co-operation, DG Environment and the Joint Research Centre of the European Commission are developing European guidelines for measuring the Environmental Footprint of products (covering goods and services) and organisations.
The objective is to support decision-making processes in business and policy with a comprehensive multi-criteria set of indicators based on the robust and quality assured measurement of environmental performance.
The documents provide guidance on how to calculate a Product Environmental Footprint (PEF) and an Organisation Environmental Footprint (OEF), as well as how to create product category or sector specific requirements for use in Product Footprint Category Rules (PFCRs) or Organisation Footprint Sectorial Rules (OFSRs).
Each requirement in the PEF and OEF guidelines has been chosen taking into consideration the recommendations of existing environmental accounting methods. Although existing methods align on some of the guidance they provide, discrepancies and/or lack of clarity remain on a number of important decision points, which significantly reduces the consistency and comparability of the results. In some cases, it was necessary to go beyond the level of guidance provided in existing documents. An example is the coverage of impact categories and the models used for calculation.

For the selection of relevant impact categories, a "default list"of 14 midpoint Life Cycle Impact Assessment (LCIA) categories is provided together with models and characterisation factors. The default list is based on the International Reference Life Cycle Data System (ILCD) Handbook recommendations for LCIA. If it can be demonstrated that a certain impact category is not relevant for the product or organisation under study, it can be neglected. If it can be demonstrated that other impacts are relevant or that for a specific impact category a better model is available, this information can be provided under "additional environmental information". However, for comparability reasons, the impacts have to be calculated as "baseline"according to the model from the default list.
In the creation of the guidelines, the right balance had to be found between different objectives. For instance, to ensure a more robust and reproducible decision support compared to existing approaches, comparability was often given priority over flexibility. A balance also had to be found between latest scientific developments and practicability and required efforts.

RA05 - Classification and risk assessment of metals and inorganic substances

RA05-1

Speciation in the transformation/dissolution examination of tungsten and antimony metal and compounds

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Speciation is held to be a key factor in the human health and environmental effects of metals in solution. In this study, we present the results of the examination at pH 6 and 8.5 of the T/D (Transformation/Dissolution) characteristics of W (tungsten) metal and several of its compounds, measuring the concentrations of total dissolved W and the tungstate ion, WO_4^{2-}. We have also determined the T/D behaviour of Sb (antimony) metal and several of its compounds with respect to total dissolved Sb, and for the 1 mg/L loadings, the speciation of dissolved Sb(III) and Sb(V). We show how the T/D data have been used to derive UN GHS (United Nations Globally Harmonized System of Hazard Classification) or EU CLP (Classification, Labelling and Packaging) outcomes. We used high performance liquid chromatography and inductively-coupled plasma mass spectrometry to analyse for the corresponding dissolved species. For the W compounds examined, the T/D data revealed that all dissolved W existed as WO_4^{2-}. $Na_2WO_4.2H_2O$, ammonium para- and meta-tungstate were readily and completely soluble, yielding measured W concentrations of about 67 mg/L, and WO_4^{2-} concentrations in the range 75 to 93 mg/L with 100 mg/L loadings, which correspond to all W dissolved as WO_4^{2-}. Compared to an acute ERV (Ecotoxicity Reference Value) of 31 mg/L, their 168-hr T/D concentrations would classify $Na_2WO_4.2H_2O$, APT, AMT, WO_3 and $WO_{2.9}$ as GHS Acute 3, but would not classify them under the EU CLP scheme. W metal and tungsten carbide would not classify under either scheme. Regarding $NaSb(OH)_6$ and Sb_2O_3, Sb dissolved entirely as Sb(V) and Sb(III), which are its respective valences in these compounds. With Sb metal, Sb dissolution was primarily as Sb(III). For Sb_2S_3, the speciation data suggested a significant degree of Sb(III) oxidation to Sb(V) over 28 days. For $NaSbO_3$, Sb dissolved as Sb(V), since antimony is pentavalent in this compound. For $Sb_2(C_2H_4O_2)_3$, the $C_2H_4O_2^{2-}$ ligand appeared to stabilize Sb(III) in solution, with only a moderate amount of oxidation. Similar comments apply to the CH_3COO^- ligand in $Sb(CH_3COO)_3$, particularly at pH 6. On the other hand, Sb(III) released from $SbCl_3$ was readily oxidized to Sb(V). With pentavalent Sb in Sb_2O_5, the speciation data indicated an initial small amount of Sb(III) that oxidized to Sb(V) over the 28 days. A comparison of the T/D data with the 6.9 mg/L acute ERV for dissolved Sb revealed that none of Sb metal and its compounds would classify under the EU CLP.

RA05-2

Transformation/dissolution of copper alloys: comparison of two anti-abrasion devices for massive sample testing

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In view of deriving the environmental classification of copper alloys, the potential for metal releases from a range of copper alloys was assessed using the OECD Transformation/Dissolution (TD) test (2001).
Metal releases from metals in massive and powder forms are a function of the surface area exposed to the media. Consequently, to assess comparative metal releases from copper alloys, there is a need to standardize the surface area exposed and to preserve the integrity of the surface as well as the corrosion and passivation layers formed. The aim of this study was to define a protocol suitable to TD testing of massive forms of copper alloys.
Accordingly, two anti-abrasion devices were designed to protect the integrity of the alloy samples. The first device involves two polypropylene (pp) wheels attached to the ends of an alloy wire sample, to avoid metal contact with the vessel walls. The second device is an epoxy jacket mounted around the sample; in this case the alloy surface exposed to the media was polished to assure a known and homogeneous surface quality and avoid effects of corrosion and passivation, proper of sample aging under uncontrolled environmental conditions.

The non-abrasion devices were applied to nine different copper/zinc and copper/tin alloys and the samples were subjected to 7 days TD at pH 6.
The T/D results of samples embedded in epoxy resin showed lower experimental noise compared to those for the polypropylene wheels and is therefore considered as a more appropriate methodology for transformation/dissolution testing of massive forms.
Microscopy studies of samples surface concluded that defects in the alloy surface during the wire production were responsible for the higher variability in the T/D results of the polypropylene wheels protocol, compared to the epoxy polished mounted sample protocol.
The surface-specific metal releases from the alloy samples, using both anti-abrasion protocols, usually increase linearly with time, with faster dissolution rates for lead and zinc and lower rates for copper and nickel. The dissolution kinetics of lead in three samples, demonstrate a decrease in the metal release ratio as the tests progress, suggesting a depletion of lead from the alloy surface. For copper, the main component of the alloys, the dissolved copper concentrations measured in the alloy were between 0.04 and 2.05 $\mu g/mm^2$, compared with the values observed from pure copper samples (0.14 to 0.41 $\mu g/mm^2$).

RA05-3

Transformation/dissolution of copper concentrates: effect of mineral composition on metal solubility

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In view of deriving the environmental classification of copper concentrates, being complex, heterogeneous and variable inorganic substances, this study aims at understanding the relation between the elemental/mineralogical composition of some selected copper concentrates and the Transformation/Dissolution behaviour of these concentrates.
The total elemental composition of five copper concentrates, obtained from different copper ore bodies and assessed demonstrated the presence of Cu, Fe, Zn, Pb, Cd, Co, As in various concentrations. The mineralogy of the samples, determined by X-ray diffraction and microscopy studies, revealed the presence various copper minerals: Bornite, Chalcocite, Chalcopyrite, Covellite, Digenite, Enargite and Tennantite.
The release rates of Cu, Pb, As, Zn, Co and Cd from the five copper concentrates and the 7 minerals identified in the copper concentrates were subsequently assessed, during short term (7 days) Transformation/Dissolution tests (TD) at pH 6 and a loading of 100 mg/L, in accordance to the OECD Transformation/Dissolution protocol (TDp) and the standard operating procedure.
The results demonstrate that during TD, especially copper, lead, zinc and arsenic and sometimes cobalt and cadmium are released from the concentrates. Relatively lower release rates were observed for copper and arsenic (0.2-4%) and the highest release rates were observed for lead (7- 35%). The detailed kinetics from the T/D tests show that the metal release rates generally decrease as a function of time.
Copper releases from copper minerals are lowest for Chalcopyrite (0.3% copper release during 7 days TD) and highest for Chalcocite (5 % copper release during 7 days TD). From the data, it can be concluded that it will not be possible to derive one release or one environmental classification entry applicable to all copper concentrates. Comparison of release data among concentrates and their mineralogy clearly indicate that the metal release rates depend on the elemental and mineral composition of the copper concentrate. The results further indicate that, as demonstrated for copper, that the metal releases from copper concentrates can be predicted from the mineral composition and the mineral- specific metal releases. The releases of lead remain difficult to interpret.

RA05-4

Metal classification using a unit world model: assessing removal rates from the water column and remobilization from sediment with TICKET-UWM

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European Union (EU) regulations pertaining to Classification, Labelling, and Packaging (CLP) of chemical substances follow the United Nations Globally Harmonized System (UN GHS). Under this system, speciation, partitioning, and precipitation are recognized as critical elements in metal hazard classification. Guidance on environmental transformation of metals provided in the EU CLP guidance document includes a provision for demonstrating removal from the water column to assess the "persistence"or lack of degradation of metals. In analogy to organic chemicals, "rapid degradation"for metals requires greater than 70% removal within 28 days. However, unlike organic chemicals, where removal from the water column occurs via degradation, metal removal occurs through changes in speciation (partitioning and precipitation) followed by sedimentation which transfers metal to the sediment. Therefore, in line with the GHS guidance, "rapid degradation"for metals requires one to demonstrate not only rapid loss from the water column, but also limited remobilisation potential from sediment.

A unit world model for metals in lakes, TICKET-UWM, has been developed that considers key processes affecting metal transport, fate, and toxicity including complexation by aqueous inorganic and organic ligands (e.g., DOC), adsorption to particulate organic carbon (POC), binding to biological receptors (biotic ligands), and transport of dissolved metals and solids between the water column and sediment. The TICKET-UWM was used to assess the rate at which metals (Cu, Pb, Zn, Ni, Co, and Cd) are removed from the water column in a generalized lake system through partitioning and settling. The model was also used to assess metal speciation changes in the sediment and the potential for metal remobilization from sediment.
Model results indicate that, in most cases tested, greater than 70% of the metal added to the water column was removed within 28 days. Results also suggest the potential for remobilization of metals is limited, particularly when acid volatile sulfide (AVS) is present to precipitate metals as metal sulfides.

RA05-5
A BLM probabilistic approach to integrate variability in the derivation of Water Quality Criteria at regional and local scales
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The biotic ligand model (BLM) is one of the more promising models allowing to derive Water Quality Criteria (WQC) based on true bioavailable fractions of metals. However, several physico-chemical parameters must be assigned for running BLMs (i.e. pH, major cations, DOC) and the operational use of BLMs can suffer several flaws because of:
(i) the lack of comprehensive data. National monitoring programs of water bodies were indeed not originally designed for BLMs application and, as a consequence, some datasets can be incomplete;
(ii) natural variability. Rivers and lakes can indeed show great spatial and temporal variations. So far however, only single values were generally considered for describing variables of concern, and the high natural variability with time and along a river watershed was ignored.
The main objective of this study was then to investigate the potential of probabilistic approaches able to capture the uncertainty of variables of concern and the incompleteness of datasets for BLMs application on large scales. The methodology was tested on the Loire river watershed for copper, where different spatial scenarios were considered.
Data needed for running the selected BLM model were extracted from the database freely put available on the web by national Water Management Agencies. Considering all data available for pH, DOC and Ca concentration, normal Probability Density Functions (PDFs) were fitted.
Data available for copper showed that a significant fraction of dissolved concentrations (about 50%) were below the limit of detection. In order to impute realistic values to these non-detects, 'distributional' methods were used. In addition, probabilistic risk assessment was also conducted at local scale (i.e. considering data collected at a given monitoring station only). In such a case, the number of available data can be reduced dramatically and frequentist statistics can be more subject to criticism. To overcome the problem of data scarcity, a Bayesian approach was proposed.

Results showed that PNEC values calculated with or without probabilistic approaches significvantly differ, e.g. if non-detects are ignored, the risk index is above one (situation at risk), while it is below one if a distributional approach is considered (situation at no risk). Similarly, in case of scarcity of data at local scale (i.e. at a given monitoring station), frequentist and Bayesian approaches led to results significantly different.

RA05-6
Accounting for both local aquatic community composition and bioavailability in setting local quality standards for metals
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Recent years have seen considerable developments in the ability to make water quality standards for trace metals more ecologically relvant by taking account of the effect of local water chemistry conditions on bioavailability. This prevents situations where a different level of risk is considered to acceptable at different sites due to changes in bioavailability which are not accounted for in the standard. We describe preliminary efforts to address an additional issue in the development of water quality standards which are specific to particular locations, by taking account of the composition of the local ecological community (the ultimate protection objective). This has occasionally been addressed through the use of field measurements to derive species sensitivity distributions (SSD) in sediments. An alternative approach, which combines a quality assessed ecotoxicity dataset with field measurements of the abundance of benthic macroinvertebrates to derive an SSD based on the community which is either expected to be present, in the absence of anthropogenic pressures, or the community which is present at the sites. Site specific standards are derived for zinc in an area impacted by historic mining activities. Site-specific targets for zinc, based on the macroinvertebrate ecology predicted or observed at a site, can be derived and can result in improved compliance compared to the use of both conventional and bioavailability-based EQS. In addition to zinc, the approach is likely to be applicable to other metals and possibly other types of chemical stressors (e.g. pesticides). However, the methodology for deriving site-specific targets requires additional development and validation before they can be robustly applied during surface water classification.

RA06 - Contaminated sediments in a changing environment

RA06-1
Bioavailability and beneficial use as primary demands for a management guidance of contaminated dredged sediments
F.A. Ahlf, B. Wirska, A. Scheffler
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Management of contaminated sediments is a key issue in order to establish a sound development of the Baltic Sea and contributing to the EU Strategy for the Baltic Sea Region (EUSBSR). This issue is of utmost importance according to Helcom and addressed by the BSR funded project SMOCS (Sustainable Management of Contaminated Sediments). The main delivery of SMOCS comprises a guideline, including tools for assessment of sustainability, and decision support.
The purpose of this lecture is to present the draft guideline on sustainable management of contaminated sediments for dredging projects all around the Baltic Sea. This proposal is a result of the joint EU-project SMOCS under consideration of actual national and international regulations, integrating other projects as well as interests of stake-holders. For example, the participants of a workshop preferred a guidance document giving new ideas and an overview of options for dredged material management. Exact definitions for the condition of dredged material (when to call dredged material "clean", "contaminated"or "hazardous") and action levels were required.
Emphasis was given to fulfill political demands as to avoid waste production. Therefore it was primarily recommended to assess the feasibility of beneficial use of the sediments. Bioavail¬ability concept for the derivation of sediment quality standards has a challenge to foster this approach, because not the total amount of contaminants is of importance rather than the biological available part. Such risk assessment based on laboratory or in situ studies meets the request of the European Water Framework Directive to develop a toxicity-based bioavailability model to estimate the risk of sediment-associated contaminants.
The purpose of an LCIA probably in combination with a Risk Assessment is to ensure that dredging activities are performed in an environmentally acceptable manner, use sound engineering techniques, which they are economically warranted and take sufficient consideration of long term effects. The choice of appropriate indicators is given in detail as part of a Decision Support Tool.

RA06-2
Natural attenuation in sediments
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Due to polluted groundwater in urban areas, sediments in urban water streams become polluted as well. This can cause pollution of surface waters. Natural attenuation of chlorinated hydrocarbons in sediment can be used to sustainably manage or remediate groundwater pollution. Due to the change in remediation procedures in the Netherlands from site specific remediation to area specific remediation, an approach based on natural attenuation will be increasingly considered. Provided that the risks of this approach can be controlled, natural attenuation processes in sediment can be a valuable contribution to area specific management and remediation plans.
However, there are still some knowledge gaps about these natural processes. Also research methods to quantify these processes are lacking. And the possible ecological effects in sediment or surface waters are still unknown.
From the knowledge gaps, research questions have been defined. Hoe are the most important processes related and can these processes be modeled? Where does biodegradation occur? How fast is this process? Can it be stimulated? Which techniques can be used for monitoring?
Six polluted sites in three cities in the Netherlands were sampled, including 1 reference sample per site. Samples were either frozen in liquid nitrogen or the individual sediment layers were sliced and sampled in the field. Chemical and molecular (Q PCR) analyses have been performed in order to characterize the sludge and sediment.
The first prelimary results show that in the toplayer of the sediment, which contains the highest organic matter content, anaerobic conditions are present. In this layer the microbial activity is higher than in deeper sediment layers. The dechlorinating capacity in this layer is higher than in deeper layers. However, in the toplayer, not only anaerobic organisms are present, but also aerobics and micro-aerophilics. This implies that microaerophilic conditions are present and chlorinated ethenes can be both anaerobically and aerobically be degraded. In the deeper layers the dechlorinating capacity is lower. This has implications for dredging managent in this specific canal. Dredging of the canal would, at least temporary, decrease the dechlorinating capacity. This could cause an increase in chlorinated ethenes in surface water and result in ecological risks during a certain period of time. The rest of the results will become available in December and January.

RA06-3

Assessing the impacts of climate change on the fate and transport of HCB and Cd in the Elbe River Basin

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Sediment-sorbed concentrations of Hexachlorobenzene (HCB) and Cadmium (Cd) in sections of the Elbe River basin significantly exceed maximum allowable concentrations established by the European Commission. Even though concentrations of both contaminants have decreased significantly over the past 15 years, levels remain elevated. In addition, previous studies have documented that downstream transport of contaminated sediment occurs primarily during high water events. Given anticipated climate-change induced changes in mean discharge, potentially including an increase in the magnitude of high and low water discharge events, this study seeks to evaluate the role of climate change in mediating the long-term fate and transport of HCB and Cd in the Elbe River basin. To better understand the transport of cohesive sediments and associated contaminants, a hydrodynamic and cohesive sediment transport model for a 230 km segment of the Middle Elbe River was developed. Of particular interest is contaminant transport to floodplains and retention time in the numerous groyne fields that line the banks of the Elbe River. Multiple climate change scenarios involving changes in the amplitude and phase of yearly streamflow were used to simulate contaminant transport throughout the Elbe River basin at 25 and 50 years in the future. Integration of modeling output with the results of recently collected (2010, 2011) sediment data enabled an enhanced understanding of current and potential future dynamics of HCB, Cd and cohesive sediment in the Elbe River. Modeling results, challenges simulating transport in groyne fields, techniques for resolving data gaps, and broad-scale suitability of the model to European river basins are discussed.

RA06-4

Dioxin-like activity of sediment samples from the Elbe River and soil samples from the Elbe associated flood area

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While the water quality of many European streams improved, sediments as sinks and secondary sources of persistent organic pollutants (POPs) are underestimated by the EG-Water Framework Directive. The aim of the present study was to compare the dioxin-like activity of Elbe River sediments and soils of the associated flood area.
Sediments from the year 2008 originated from Czech and German river sections and from the North Sea and were considered to reflect the present pollution of the Elbe River. In contrast, the soil samples of the Elbe associated flood area - taken after the Elbe flood of August 2002 - rather represented a remobilization potential of POPs during big floods. These samples originated from three transects, located downstream, upstream and close to the confluences of the Elbe tributaries Mulde and Saale. Hence, they also might indicate the influence of the tributaries on the contamination of the Elbe.
All freeze-dried samples were extracted by means of pressurized liquid extraction. Dioxin-like activities were determined via the EROD assay with RTL-W1cells and in parallel via the H4IIE-luc assay with the eponymous transfected rat hepatoma cell line. All samples showed elevated dioxin-like effects, except two North Sea samples, showing no effects in the H4IIE-luc assay. Nevertheless, both bioassays gave a good correlation with Bio-TEQs between 1307 and 10462 pg/g dw. They identified the industrial city Lysa nad Labem as the highest contaminated site and revealed the floodplain soils to be equally contaminated like the Elbe sediments. But a flood influence could only be supposed due to the missing pre-flood data and a soil sampling depths that gave no information about freshly deposited matter during the flood 2002. An influence of the Elbe contamination through its tributaries could not be found. A comparison of Bio-TEQs with their respective Chem-TEQs for the sum of polychlorinated dibenzo-p-dioxins (PCDD/F) and dioxin-like polychlorinated biphenyls (DL PCB) was performed. The Chem-TEQs accounted between 0.1 % and 11.9 % for the observed Bio-TEQs. Lower percentages were found for sediments than for soils, indicating that PCDD/F and DL-PCB are more important for the floodplain contamination.
A multilayer fractionation of three selected transect samples, which eliminated the moderately persistent pollutants, gave clear evidence that the majority of dioxin-like activity in these samples was caused by non priority and non-persistent pollutants.

RA06-5

Can flood events affect rainbow trout? The biomarker-cascade after exposure to PAHs in sediment suspensions

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In context of the ongoing scientific discussion about the potential ecotoxicological impacts of flood events, it is important to understand the detailed mechanisms of contaminant uptake from suspended particles and related effects on aquatic biota. As part of the interdisciplinary project Floodsearch II, rainbow trout (*Oncorhynchus mykiss*) were exposed to suspensions of natural sediment from the River Rhine (Ehrenbreitstein Harbour). Prior to suspension, the sediment was spiked with the polycyclic aromatic hydrocarbons (PAH) pyrene, phenanthrene, chrysene, and benzo[*a*]pyrene at environmentally relevant concentrations (4.1, 5.0, 3.3 or 8.3 mg kg^{-1} dry weight, respectively). A control treatment without addition of PAHs was also included in the experimental design. The experiment was conducted first at an average temperature of 24 °C and repeated at 12 °C. The nominal concentration of suspended solids was 10 g L^{-1} in both experiments. After 0, 1, 2, 4, 6, 8 and 12 days of exposure, physicochemical parameters, concentrations of PAHs in suspended matter, as well as biomarkers of exposure in rainbow trout (biliary PAH metabolites, hepatic 7-ethoxyresorufin *O*-deethylase (EROD) activity and lipid peroxidation) were measured. Instrumental chemical analyses revealed that concentrations of pyrene and phenanthrene in suspended solids decreased over time, while no significant degradation was observed for chrysene and benzo[*a*]pyrene. Concentrations of biotransformation products of PAHs in bile of fish increased slightly in the treatment without addition of PAHs at 24 °C, while average levels increased to 166 µg ml^{-1} for 1-hydroxypyrene (control value 4.6 µg ml^{-1}) and 17 µg ml^{-1} for 1-hydroxyphenanthrene (control value 0.1 µg ml^{-1}) in the spiked treatment within two days, followed by a decrease. In the 12 °C experiment, uptake of PAHs was slower. With a latency of two days, the peak of metabolism in the 24 °C experiment was followed by a peak of lipid peroxidation that indicates oxidative stress caused by PAH metabolization. EROD was not significantly induced by the treatments. Significant differences were observed between the bioavailability of freshly spiked and field-aged PAH contamination. The results of this study indicate the importance to account for the temporal variability of biomarker responses in sediment suspension experiments to comprehensively assess the biological effects caused by particle-bound pollutants.

RA08 - Escape from the Ivory Tower - Environmental sciences should impact public and policy

RA08-1

The gap between scientific publication and the press - a case example

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Nanomaterials are of common interest for industry as promising novel technologies, but they are also of certain public concern due to lack of knowledge about their effects for health and environment. Results of our study on effects of carbon nanotubes (CNT) on green algae were published in 2011 in the peer reviewed journal *Environmental Science & Technology* [1]. The major findings of our study were that CNT inhibited growth of green algae, but not due to direct effects, like reduced photosynthetic activity of the green algae, but mainly due to indirect effects, namely shading of light in turbid test suspensions and agglomeration of the CNT with algal cells. After the scientific publication in fall 2011, we published a press release which surprisingly evoked a vast number of reactions in the media, the common public, the institutes involved, and a smaller number of reactions in the scientific community. The press discussed the results very diversely: Taking over our message to interpretations far away from the scientific facts presented in *ES&T*. Examples for headlines are (Translated from German): "Nanotubes as Growth Inhibitors - Toxicity Tests with Green Algae"[2], "Nanoparticles Identified as Potential Environmental Killers"[3], and "Nano-Waste Could Disturb Aquatic Life"[4].
The lessons learned from this case study are a) that news on topics of public concern such as toxicity of CNT and engineered nanomaterials are very closely monitored and instrumentalized both by the pro- and the anti-nano community for their respective intentions, and b) therefore, reactions on press releases concerning these topics have to be monitored closely, wrong quotations must be corrected and biased interpretations must be adjusted, in order to provide correct scientific information for the common public.
[1] Schwab F, Bucheli TD, Lukhele LP, Magrez A, Nowack B, Sigg L, Knauer K. 2011. Are carbon nanotube effects on green algae caused by shading and agglomeration? Environ Sci Technol 45:6136-6144.
[2] Speicher C. 2011. Nanoröhren als Wachstumshemmer. Neue Zürcher Zeitung (NZZ), Zurich. Nov 9 edition.
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[4] Kurt de Swaaf. 2011. Nano-Müll könnte Leben im Wasser stören. www.spiegel.de/wissenschaft/technik/0,1518,797102,00.html. Accessed 30 Nov 2011.

RA08-2

Discourse of risk communication - taking the risk of communicating risks

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Risk communication, especially to the general public and end users of plant protection products, is an important challenge. Currently, much of the risk communication the general public receives is via the popular press, and risk managers face the challenge of presenting their decisions and their scientific basis in an understandable way. Therefore, we decided to explore the obstacles in risk communication, as done by expert risk assessors and managers. Using the discourse analysis framework we have studied perspectives of three stakeholder groups - regulators, industry representatives and academics across Europe.
We conducted 30 confidential interviews, which comprised 15 open-ended questions. A part of the interview guide was focused on communication of pesticide risk to the general public and the ideas experts in the field of risk assessment/management hold of the public perception of pesticides. We employed the key informant approach in recruiting our participants. They were first identified as key stakeholders in ecological risk assessment of pesticides and then sampled by means of a snowball sampling.
The most visible motif we identified in the preliminary analysis was a strong disconnect between "emotions"and "science"in communicating risk. These two were seen as opposites, with "science-based"risk communication perceived as superior to the "emotion-based"communication. The latter was presented as detached from facts and related to political sensitivities.
Our results show that despite the attempt to polarise emotion-based and science-based communication, emotionally-charged language and reactions are always present in risk-related topics. Our preliminary findings suggest that there needs to be a balance of "emotions"and "science"in communicating risks - the discourse of risk is tightly related to emotional reactions. Moreover, studies into risk perception found that emotional reactions often plays a more significant role in perceiving risks than our cognitive judgement. Whilst it is important to keep the process of risk assessment objective and science-based, the general public can be better informed from communicating risks with the costs and benefits clearly outlined, and emotional connotations are easy to understand. Emotionally-charged messages have been successfully used in health risk communication (e.g. fear appeal) and public awareness campaigns. It seems that risk assessors and managers can also learn from these examples.

RA08-3
Reach Regulation: communication behind the inforamtion needs
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Reach Regulation : Communication Behind the Information Needs.
The implementation of REACH aims a high level of protection of human health and the environment . Industry has the burden to prove the safety use of products and to ensure control of any risk. If the information to public is also one of the major goals of the regulation, the first steps of implementation show different ways to experience information diffusion.
These works were conducted in the framework of a research project « How to use REACH. How the stakeholders approach REACH through technical classes'. Discussion meetings have been organised with the parties who have designed the regulation and who are assuming the control of its implementation, but also people who are implementing REACH in professional organisations and private companies : Reach regulation designers, chemical producers, chemical industry trade-unions , state-member representative. Information on/into REACH, at this early stage (registration) , is not a simple question and REACH proceeds by 'Learning by doing ». Information on REACH and products is circulating to some extend into topical focused forums (SIEF) and into chemical consortia, but it appears that different stakeholders don't share the same points of view (what kind of questions for which recipients?). Communication to public which is also an important objective of the regulation is far beyond what maybe expected at that stage. The next steps (evaluation, authorization) surely need to plan communication towards the public , outside from the closed and confined space of acting stakeholders.

RA08-4
Research findings and decision making: the case of renewable energy
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Scientific research can have a role in the promotion of more sustainable patterns of consumption and production because it can provide information aimed to raise awareness about the impacts of different behaviours and to support more sustainable choices from different kind of actors. The challenge posed to science in this context is to provide information that is effectively supporting for decision making processes at different scales and that can be easily understood by all the stakeholders involved in the process (policy makers, entrepreneurs and citizens). In recent years the attention of citizens on the issues of sustainability, environmental impacts and sustainable behaviour has grown considerably [1]. In parallel the demand for scientifically sound and transparent information upon which to base consumption choices and behaviours is growing among citizens.
Nonetheless, it is difficult to think that there may be a direct contact between those who do research and who makes the decisions: firstly, because in most cases there are no opportunities for direct contact (e.g. to citizens) and, secondly, because is necessary to translate the information resulting from scientific research in a language that is understandable. The lack of on communication between science, policy and citizens communication can lead to not evidence-based decision making, lack of trust and unsustainable behaviour due to low level of information and awareness. One possible way of success in environmental communication could be represented by the presence of those intermediaries who have relationships with key stakeholders and are able to translate information for them so that they become understandable and translatable into action.
We present a discussion about wood use as a renewable energy source: communication of the main scientific findings about its sustainability and environmental impacts associated to it in support to decision making in energy planning and energy use.

RA08-5
Challenges of integrating science and people within a network of excellence
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A Network of Excellence (NoE) was recently formed in radioecology, a science concerned with the transport and effects of environmental radiation. The NoE was formed to combat several problems in radioecology that are not uncommon in many other disciplines: 1) a steadily decreasing funding base; 2) fragmentation of resources and infrastructures; 3) poor recruitment of young scientists; and 4) retirement of key personnel. Nine organizations from eight countries formed the NoE with goals of developing a sustainable, long-term integration of radioecology in Europe. The integration that was required by the scientists resembled, in the business world, a partial merger of divisions from within different organizations. We thus sought a business school that specialized in change management to help us with the integration. Our NoE became a special project for five of MBA students. This presentation highlights some of their findings. Foremost, the MBA team determined that to create a sustainable NoE, there had to be integration among the people. This included working towards a shared vision, understanding the cultural differences involved in the project , and sharing the same expectations about what the scientists as individuals and their respective organizations receive from the NoE. Studies from past attempts at mergers and acquisitions in the business world indicate that failure to integrate usually occurs because the fundamentals of change management are overlooked and/or taken for granted.
[NOTE to organizers: This platform session is intended for a special session organized by F. Brechignac and I. Linkov, (francois.brechignac@irsn.fr). I do not see it listed among the 'topics'. Although the subject of this presentation seems to fit perfectly with SETAC's conference theme of Integrating Science and People, I do not see where it might best fit among your topics. Below, I have listed F24....but welcome your suggestions as to other options. Thank you.]

RA08-6
Keep your boots muddy
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The German Federal Environment Agency runs a site for aquatic simulation in the very south of Berlin, which also includes a set of outdoor and indoor artificial pond and stream mesocoms (FSA) for ecotoxicological research (http://www.umweltbundesamt.de/wasser-und-gewaesserschutz/fsa/). Up to the present, 30 studies were carried out in that facility during the last 10 years. The results have been popularised via the official homepage, guided tours, conference posters, talks and sessions, scientific journals, magazines, newpapers, and TV features. In search for further means to reach a wider audience apart from ecotoxocological professionals and people interested in natural sciences, the idea of the artist Anne Rinn (www.anne-rinn.de) to stage an exhibition and to create a film entitled 'Keep Your Boots Muddy' was supported by the FSA team. Both exhibition and film pivot on the triangle nature-simulation-art with simulation trying to create artificial nature. The presentation will be the 10 minutes version of the German film with English subtitles.

RA09 - Focal species of birds and mammals and their ecological behaviour for refined risk assessments of plant protection products in Europe

RA09-1
Benefits of 'EFSA Risk Assessment for birds and mammals' guidance document for ecological refinements
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EFSA, Parma, Italy
In order to gain EU Level approval of an active substance under Regulation (EC) 1107/2009, and previously EU Directive 91/414/EEC, it is necessary to assess the risk to bird and mammals. Since the early 2000's to 2009 the main guidance document used was the 'SANCO/4145 Guidance Document on Risk Assessment for Birds and Mammals Under Council Directive 91/414/EEC', European Commission (2002) (hereafter referred to as SANCO/4145). However, in 2009 the European Food Safety Authority (EFSA) issued a new guidance document ('Risk Assessment for Birds and Mammals', EFSA (2009)) which aimed to update and improve bird and mammal risk assessment in the EU. Both guidance documents follow a tiered risk assessment whereby a first tier risk assessment seeks to address low risk situations. However, should a first tier assessment fail to be sufficient to demonstrate a low risk then it is necessary to refine the risk. There are various approaches outlined in both guidance documents including the use of ecological data. The presentation will outline the key differences between the two guidance documents and highlight the benefit of risk assessment methodology in EFSA (2009) in relation to ecological refinements. An analysis of a hypothetical case will demonstrate how the first tier risk assessment in EFSA (2009) provides valuable information for the refined assessment. An example will be given to show how improvements in the use of ecological data and uncertainty analysis will be used in the overall characterisation of the risk.
Improvements to first tier risk assessment methodology in EFSA (2009) result in a much more informative assessment. Further guidance is also given in conducting and interpreting ecological field studies and utilising the literature. It is hoped that this will aid the development of more robust risk assessments and consistency in evaluation. A further improvement is that it is necessary to conduct a risk characterisation and uncertainty analysis for every refined risk assessment. It is anticipated that this will improve communication of the risk as well as allowing risk assessors to make best use of the available information in a scientific manner.
The new EFSA guidance document will help applicants and risk assessors to produce reliable, robust and informative risk assessments. It provides more clarity at the first tier, for refined assessments and for the overall communication of the risk.

RA09-2
Risk assessment of birds and mammals exposed to plant protection products in the Nordic and Baltic countries
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Regulation EC 1107/2009 regarding placing of plant protection products on the market in EU entered into force 14 June 2011. A central aspect of the regulation is the principle of mutual recognition within zones with comparable conditions. To facilitate work-sharing within the Northern zone, the Nordic and Baltic countries have regular meetings to harmonize risk assessments. Agreements among the countries are compiled in a guidance document for the Northern zone which is available at the authorities' homepages.
To harmonize initial risk assessment of birds and mammals, the Northern zone has agreed on using the EFSA Guidance document (EFSA Journal 2009; 7(12):1438). If initial assessments indicate potential risks, refined risk assessments can be provided. Refinement options include which species that could be used (focal species) and the ecology of these species, e.g. proportion of diet obtained from treated area (PT) and composition of diet obtained from treated area (PD). Other refinement options consider the properties of the substance, e.g. degradation time in/on treated crops and weeds (foliage DT50).
To harmonize a refined zonal risk assessment, the Northern zone has agreed upon the following:
Default foliage DT50 used in initial risk assessment could be replaced if results from at least 4 study sites are available. If results from 4-10 sites are presented, the longest DT50-value should be used. If more than 10 values are available, the mean value can be used. Residue decline studies may only be used for refinement of DT50 if results are evaluated according to the EFSA guidance document.
Default PT (100%) could be replaced by referring to studies including, as a minimum, 10 individual animals. The 90'percentil PT value from these studies should be used in the refined risk assessment. Studies to refine the PT may only be used in the risk assessment if they are evaluated according to the EFSA guidance document.
Focal species and their PD and PT will be harmonized, as far as possible, for major crops within the zone. Such guidance will enhance uniform and agreed refined assessments and ease evaluation of registration reports. Our goal is that this guidance for refined risk assessment will be available in May 2012 when the SETAC conference is held.
Modelling (body burden or ecological models) are not considered appropriate for higher tier risk assessment until validated models and guidance are available.

RA09-3
Identification of bird focal species in France for refined risk assessments for plant protection products
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The refined risk assessment for birds and mammals might be based on different parameters such as measured residues in food items, and/or on behaviour and diet of focal species. The EFSA Opinion (2009) provides generic focal species for the major crops, but when further refinement is necessary, focal species defined in the opinion as "real species that actually occur in the crop when the pesticide is being used"should be identified. The National Museum of Natural History in France has got a huge data base containing registrations of bird presence on the territory, based on field observations made by a large network of naturalists. A methodology has been built to identify the focal species on several groups of crops by crossing the information issued from the Museum database, the repartition of crops in France, protected studies provided by industry, and a literature review. The outcome of this work, presented as a compiled document, contains identified focal species per groups of major crops, their behaviour and feeding habits.

RA09-4
Bird focal species in crops according the EFSA - how to find the right candidates
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According to EU Council Directive 91/414/EEC and Regulation 1107/2009, the effects of crop protection products on wild mammals and birds have to be assessed. For this reason crop-specific focal species candidates can be defined for different periods representing different BBCH growth stages. The total data base consists of 72 field studies of plant protection product producing companies who register their products within Europe (BASF, BCS, Cheminova, DOW, GOWAN, Makhteshim, Irvita, Isagro, Monsanto, Sharda and Syngenta). The studies have been conducted in eight different countries spread across member states in the central and southern registration zones of Europe. The total period during which the surveys of each study took place ranges from a minimum of two weeks to up to four months. Here we will present data of two crops (cereals and pome fruit), and the most important value calculated on the basis of the raw data is the frequency of occurrence per field (FOField), which denotes the number of fields where a species was recorded as percentage of the total number of fields regardless of the number of individuals observed. Furthermore it is necessary to consider parameters such as diet guild, feeding strata, body weight and food intake rate to ensure that a given focal species are representative to provide a robust risk assessment. The focal species selection methodology is discussed using cereals and pome fruit orchards in Europe as case studies.
Acknowledgement - The authors thank all the data owners within European Crop Protection Association for access to these data and the field workers for collecting the data in the field.

RA09-5
European distributions of farmland birds used as focal species for pesticide risk assessment
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Risk Assessment guidance for birds and mammals in Europe has been described by EFSA [1]. The process is tiered. To refine risk assessment it is neccessary to define focal species in different crops at relevent growth stages appropriate for the use of the chemical applied. Focal species have been studied in 16 EFSA crop categories, mostly by Industry, in several EU member states. Here we present the data from field studies conducted by Industry. For most major crops the focal species have been determined in several MS's and this provides evidence of their distributions. Studies have not been measured in all crops in all Member States (MS) since there is room for extrapolation between zones and crops. The EU have established voluntary zonal work sharing for the registration and reregistration of plant protection products which have been described by SANCO/6896/2009 [2] stating it is reasonable to place MS in geographical zones (Zonal Approach) where there is greatest similarity in climate, crops and general conditions that may influence exposure to pesticides and hence the risk. The purpose of the presentation is to demonstrate how an evaluation of the distribution of focal species from these data can be done and to compare the distribution of focal species from these studies with the distributions for the same species provided by the European Birds Atlas database. To illustrate this approach, one crop example (cereals) will be used. The approach developed may allow extrapolation in line with the Zonal Approach, such that MS risk managers can have confidence in using refined exposure data for a single set of focal species applied to a crop within a zone or even across zones.

RA09-6

Small mammal communities in agricultural landscape in central Europe: review of long-term field data

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Little is known about general small mammal communities in agricultural landscape in central Europe. Most published data represent only a few months' data in a specific habitat type focussing on a small region. This presentation will review data from several studies performed in the last decades in agricultural landscape across different regions in Germany and the Czech Republic. Data on the distribution of small mammal species in agricultural landscape including cropped fields, meadows and adjacent field structures like hedgerows and woodland are presented. The results of three data sets in comparison will focus on general conclusions and may help to interpret the spatial and temporal composition and distribution of small mammal communities in agricultural landscape in central Europe.

RA10 - Global Mercury: Bridging science and policy

RA10-1

Mercury emissions in large Hg-polluted floodplain areas in Germany are an underestimated problem: challenges for reliable risk assessments and implications for authorities

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Environmental pollution by mercury is a world-wide problem. Particularly floodplain ecosystems are frequently affected. One example is the Elbe River in Germany and its catchment areas; large amounts of Hg from a range of anthropogenic and geogenic sources have been accumulated in the soils of these floodplains. They serve as sink for Hg originating from the surface water of adjacent river. Today, the vastly elevated Hg contents of the floodplain soils at the Elbe River often exceed even the action values of the German Soil Conservation Law. This is especially important as Hg polluted areas at the Elbe River achieve several hundred square kilometres. Thus, authorities are coerced by law to conduct an appropriate risk assessment and to implement practical actions to eliminate or reduce environmental problems. A reliable risk assessment particularly with view to organisms (vegetation as green fodder and hay production, grazing and wild animals) to avoid the transfer of Hg into the human food chain, requires an authentic determination of Hg fluxes and their dynamics since gaseous emissions from soil to atmosphere are an important pathway of Hg. However, reliable estimates of Hg fluxes from the highly polluted floodplain soils at the Elbe River and its tributaries, and its influencing factors are scarce. For this purpose, we have developed a new method to determine mercury emissions from soils at various sites. Our objectives were i) to quantify seasonal variations of total gaseous mercury (TGM) fluxes for floodplain soils at the Elbe River, ii) to provide insights into physico-chemical processes regulating these TGM fluxes, and iii) to quantify the impacts of the controlling factors soil temperature and soil water content on Hg volatilization from a typical contaminated floodplain soil within soil microcosm experiments under various controlled temperature and moisture conditions. Our study provides insight into TGM emissions from highly Hg-polluted floodplain soils in Germany and that those emissions are an underestimated problem. Current needs for reliable risk assessments, the induced implications for authorities, and future challenges will be discussed. The presented data will contribute to a better understanding of seasonal dynamics of Hg fluxes and its controlling factors. This presentation should be of large interest for a wide international audience, such as environmental scientists and managers, applied ecologists, and authorities.

RA10-2

Mercury in the Mediterranean: status and mass balance

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An interesting feature of mercury biogeochemistry in the Mediterranean is that several fish species from the Mediterranean show higher concentrations of Hg than same fish species in the Atlantic ocean, although the concentrations of total mercury in the open waters of both oceans are similar. Elevated Hg levels have been noted in environmental matrices from the Mediterranean regions adjacent to known mercury anomalies, yet, the data do not clearly indicate that the effects of these anomalies have been transmitted to open waters or to lower trophic level species living in these waters. Recent studies indicated that the main source of MeHg in organisms in the coastal areas is related to methylation in sediments, while net mercury methylation in the open ocean occurs in the water column and is linked to organic matter regeneration promoted by the presence of small-sized nano- and picophytoplankton, that dominate under oligotrophic conditions. Relatively large portion of mercury in waters is present as dissolved gaseous mercury (DGM), originating from photochemical, biologically mediated mechanisms and/or diffusion from deeper layer either due to biological and/or to tectonic activity which is typical of the Mediterranean region.

Recent studies on distribution and cycling of mercury and a mass balance were implemented. It has been shown that exchange with the atmosphere is the most important source/sink of mercury for the water compartment. Measurements have shown that the evasion of Hg varied between the different seasons with the highest evasion during the autumn and an estimate of yearly evasion from the Mediterranean Sea surface was estimated to range between 250-350 kMol/yr. Two important zones of MeHg productivity are reported in the Mediterranean Sea: one at the bottom of the euphotic layer and the other at the oxygen minimum in the thermocline.. The proposed methylation and demethylation rates vary between 0.3-6.3 % day-1 and 6.5 -25 % day-1, respectively. Based on these values the estimated production in the euphotic zone is between 500 and 1000 kMoles/yr, and degradation was estimated to 750-100 kmoles/yr. It has been shown that the total mercury exchanges at the straits are not unbalanced, while mercury entering the western Mediterranean is mainly in inorganic Hg forms and is exported to the Atlantic partially as methylated species.

RA10-3

Mercury exposure in relation to selenium and glutathione S-transferase gene deletion variants in pregnant women from Mediterranean

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It is well known that an antagonistic effect exists between selenium (Se) and mercury (Hg), and that Se can play a protective role against Hg toxicity in organisms. In order to find an evidence for such connection, total Hg and Se were determined in 1654 umbilical cord blood samples, 1081 maternal blood samples, and 1051 breast milk samples in pregnant women from Slovenia, Croatia, Italy and Greece. Methyl mercury (MeHg) was determined in approx. 30% of the samples. In addition, to observe gene-environment interactions, GSTT1 (Glutathione S-transferase theta 1) and GSTM1 (Glutathione S-transferase Mu 1) gene deletion variants were studied in a subset of 212 participating women. The study was implemented within the EU 6th framework programme PHIME.

Positive and significant linear correlation between Hg and Se was found in cord blood, maternal blood and breast milk. The strongest correlation was observed between inorganic Hg and Se in breast milk of the overall population (r=0.801). Hg and Se were found to be associated positively and significantly also in blood of Slovenian women aged 50-59 and children aged 6-11 from mercury mine area, but not in children from other areas in Slovenia, confirming the association of Se with inorganic Hg, which is the predominant species people are exposed to in the contaminated site. Se in maternal and cord blood, but not in milk, was significantly correlated with the intake of many food items in pregnancy. The strongest direct associations regarded cheese and some vegetables (artichokes and fennels). In addition, both Hg and Se were significantly associated with fish consumption, possibly explaining correlations between these two elements found in selected biomarkers. Moreover, pregnant women with homozygous deletion of GSTT1 gene showed significantly higher MeHg (but not total Hg) in cord blood compared to women with the presence of GSTT1 gene (p=0.028). When adjusted to Se levels in blood, positive and significant associations were observed also for MeHg in maternal blood. No significant differences of MeHg, T-Hg and Se concentrations between GSTM1 gene deletion variants subgroups were obtained.

RA10-4

Mercury and methyl mercury in the trophic chain of the Lagoon of Venice, Italy

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The Lagoon of Venice is one of the numerous coastal zones contaminated by mercury emitted from chemical industry (mainly alkali-chlor). Because of a long residence time of mercury, perpetually recycled between water and sediments, the transfer of mercury to biota in lagoons persists a long time after the reduction or elimination of Hg point sources. Previous studies in the Lagoon of Venice have demonstrated an elevated methylation potential, tide-driven MMHg transfer from sediments to water column and accumulation in some organisms. Here we report for the first time the initial results on Hg and MMHg bioaccumulation in the food web.

Biota and sediment samples were collected in summer 2011 in the moderately poluted northern part of the Lagoon of Venice Biota samples included pelagic and benthic

organisms from all trophic levels from primary producers to fish. Carbon and nitrogen isotopes were determined with a isotope ratio mass spectrometer (IRMS). Total Hg was analyzed using thermal combustion method (AMA 254) The Hg species were analyzed by species-specific isotope dilution and capillary gas chromatography hyphenated to inductively coupled plasma mass spectrometer .
Based on $\delta^{15}N$ results the sampled organisms covered 3 trophic levels.
Total mercury concentrations in biota varied by nearly three orders of magnitude from 0.030 µg g^{-1} d.w. (dry weight) in seagrass (Zostera marina) to 2.3 µg g^{-1} d.w. in tissue of shrimp (Palaemon elegans). There was a tendency of increasing Hg concentration with increasing trophic level, but the relation was not significant if all species were considered. MMHg concentrations varied between 5 (seegrass, phytoplankton) and about 2000 ng g^{-1} d.w (shrimps, fish) and the proportion of MMHg in total Hg was increasing with the trophic position of organisms. For the full set of data, the relation between MMHg and $\delta^{15}N$ values was best expressed by an exponential function (R^2=0.59),
On average, the accumulation of total Hg and MMHg in the organisms in a moderately polluted area of the Lagoon of Venice increased by one order of magnitude for each of the three trophic levels. However, the deviations from this rule can be considerable for benthic filter feeders (bivalve mollusks) and some fish apparently migrating from less contaminated areas. Results of this and follow up studies should provide a suitable model for risk assessment in more contaminated areas.

RA10-5
Dietary selenium at environmental concentrations reduces methyl mercury retention in some aquatic organisms at the lower trophic levels
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Methyl mercury biomagnifies along aquatic food chains and top predators - including humans with a high intake of fish or aquatic mammals - risk neurological symptoms because of the high dietary exposure to methyl mercury. Methyl mercury is taken up into organisms quite efficiently, whereas - once assimilated - methyl mercury is eliminated slowly. Thereby, the long retention times (of course together with the efficient uptake) are the main contributing factors in the biomagnification process. Selenium interacts with methyl mercury and mercury in multiple, complex and not fully understood ways. Methyl mercury contents in fish tend to be low in selenium rich (natural, manipulated or polluted) ecosystems and dietary selenium increases the elimination of methyl mercury from freshwater fish in laboratory experiments. Lower retention times in organisms at the various trophic levels will inevitably result in reduced biomagnification of methyl mercury along aquatic food chains but the role of dietary selenium on methyl mercury biokenitics in aquatic invertebrates is poorly known. The present experiments were carried out to obtain a better understanding of selenium's role for the retention of methyl mercury in aquatic invertebrates.
Dietary selenium (as selenite, seleno-cystin and seleno.methioneine but not selenate) reduced the retention on methyl mercury in the brown shrimp Crangon crangon. Environmentally relevant concentrations (< 1 µg Se/g) of selenium in the food correlated negatively with half lives for methyl mercury. Selenium in the food also reduced the retention times for methyl mercury in the marine copepod Acartia tonsa, but in a less pronounced way than in the brown shrimp. In shore crabs Carcinus maenas no effect of selenium was found.
The finding that there is a negative correlation between low, environmentally realistic selenium concentrations in the the food and the half life for methyl mercury in brown shrimps indicates that selenium may play an active role for the biokinetics of methyl mercury in the environment. This is corroborated by similar findings in zebrafish Danio rerio [1] where small increases in the selenium concentration in the food also lead to a dose-dependent decrease in the retention of methyl mercury. The potential significance of the somewhat more limited effect of selenium at the lowest trophic levels (the copepods) and lack of effect in the shore crab needs more detailed elucidation.

RA10-6
Mercury pollution in china: releases, uses and impacts
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China currently has the world's largest intentional consumption as well as unintentional environmental release of mercury (Hg). Atmospheric emissions has been estimated to about 700 tons annually, accounting for one third of the global anthropogenic emission. There are also large (but not quantified) releases to local soil and water environments. The intentional use og Hg in industrial processes and consumer products has been estimated at 1000 tons annually, roughly half of the global total.
Mercury is released to the environment by a wide range of sectors, including key industries such as mining, power generation, non-ferrous metal production, and the cement and chemical industries. The industrial use of mercury in China has caused severe pollution incidents in the past. Today, as a result of past practices, high mercury levels are found in water, soil and rice near abandoned mercury mining and smelting areas.
The presentation gives an overview of the major issues regarding China's Hg pollution issues, including releases, intentional use, environmental concentrations as well as human exposure.

RA11 - Guidance documents and guidelines for environmental risk assessment (ERA): needs, developments and progress

RA11-1
Ecological risk assessment of pesticides: linking non-target Arthropod testing with protection goals (ESCORT 3)
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The ESCORT 3 workshop (ESCORT: European Standard Characteristics Of beneficials Regulatory Testing) dealt with questions of the protection of "Non-Target Arthropods"in the context of the use of plant protection products in agriculture. It was the third ESCORT workshop that addressed this question. The Organising Committee put together a programme of discussion topics that were addressed at the workshop in plenary sessions alternating with work in sub-groups. This allowed for in-depth discussions on each of the four areas identified by the Organising Committee: a) Level of protection and testing scheme; b) Off-crop environment; c) Recovery; d) Field studies.
Approximately 60 participants registered for the workshop coming from authorities, the private sector, and academia. The participants of the workshop were assigned to one of the four sub-groups based on their knowledge and expertise, and regular plenary sessions gave participants the opportunity to comment on all areas under discussion. An opening plenary session provided background information with presentations from invited speakers. The ESCORT 3 meeting was held as a review and update of the previous meeting outputs based on current science. It also considered new issues and open points that had arisen in the interim period. The proceedings of this workshop will be finalized in the 2012 and this presentation aims at offering the audience an outline of these proceedings.

RA11-2
Development of OECD guidance on the conduct and evaluation of toxicity tests for endocrine disrupting chemicals
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The science of endocrine disrupting chemicals (EDCs) is maturing, and two jurisdictions (European Union and United States of America) have now enacted regulations for the control of these substances. It was foreseen over a decade ago that such regulations would need to be underpinned by new toxicity assays relevant to human health and wildlife species, because the more traditional suite of internationally-standardised assays was insufficiently sensitive to known EDCs. In response to this perception, the Organisation for Economic Cooperation and Development (OECD) set up its Endocrine Disrupter Testing and Assessment (EDTA) programme to develop and validate new screens with some diagnostic capability for potential EDCs, as well as tests with apical endpoints sensitive to EDCs, several of which have now been published as OECD Testing Guidelines (TG). These include 2 in vitro procedures for detecting substances with potential to affect steroidogenesis (TG 456) or interact with the estrogen receptor (TG 455); 4 in vivo mammalian assays (TG 443, 441, 407 and 440) with diagnostic capability for, and/or sensitivity to, one or more of estrogens, androgens, thyroid disrupters and steroidogenesis disrupters (so-called EATS modalities); 4 in vivo fish assays (TG 229, 230 and 234; GD 148), also with EATS sensitivity; and one in vivo amphibian assay for thyroid-active substances (TG 231). In addition, OECD has developed, or is developing, a range of lifecycle or partial lifecycle assays with birds, fish,

amphibians and invertebrates which are able to measure the apical effects of EDCs without generally being able to diagnose causality. As well as briefly describing these assays, this paper will present a new OECD Guidance Document (GD) which helps users of the assays interpret their results, assists in reaching conclusions about whether test substances possess potential or actual endocrine disrupting properties, and provides advice about a possible further testing step should this be indicated. The basis of this GD is the need to evaluate all relevant information in a weight-of-evidence approach when interpreting assays, including existing data on similar chemicals, physico-chemical properties, results of in vitro tests, and in vivo toxicity in the same and other species. It will rarely be possible to conclude that a substance is an EDC solely on the basis of a single assay, so the GD will provide much-needed assistance to chemical companies and regulators alike.

RA11-3
ECETOC Ecotoxicological assessment of endocrine disrupting chemicals
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European regulations on plant protection products, biocides and chemicals only support the marketing and use of chemical products on the basis that they do not induce endocrine disruption in humans or wildlife species. An ECETOC task force was formed to provide scientific criteria that may be used to identify and evaluate endocrine activity and disruption. This presentation focuses on wildlife species.
For ecotoxicological assessments the key considerations include specificity, potency, population relevance and negligible exposure.
Assessment of specificity is conducted within a study or species, to determine whether the endocrine mediated effect occurs at at concentrations lower than those that cause other significant toxicity. Then the evaluation proceeds to consideration of specificity in relation to endpoints obtained in other taxonomic groups, which may drive the overall risk assessment. If the adverse effects are considered not specific the risk assessment is based on the non-endocrine endpoint.
If specificity is confirmed, a risk assessment considers the endocrine endpoint with an assessment factor based on potency. The endocrine-mediated NOEC/NO(A)EL needs to be compared with other endpoints, e.g. by assessing the magnitude of the ACR, comparing the potency of the substance to a reference compound, duration of exposure that induces an adverse effect and the number of species in which the adverse effect is demonstrated
The protection goal of environmental risk assessments is the population and examples for relevant effects are: age at first reproduction, size of a reproductive event, frequency of reproductive events, duration of reproductive period, viability of young and sex ratio. Some effects are known to be responsive (and even sensitive) to, but not diagnostic of, endocrine modulation (e.g. fecundity, which can be affected by general toxicity). In such cases supporting information will be required to link the population relevant effect to an endocrine mechanism.
There are currently no specified criteria for "negligible exposure"of wildlife species to plant protection products. Based on the wording in the regulation it is evident that negligible exposure must fall somewhere between "no exposure"(i.e. nominal concentrations of 0, or less than the limit of detection/limit of quantification) and a concentration representing an acceptable or low risk.

RA11-4
Environmental Quality Criteria (EQC): a comparison of methods under different regulatory regimes
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Environmental quality criteria (EQC) form the basis for legally binding environmental quality standards (EQS). The EQC´s are derived according to different European and national legal frameworks accompanied by technical guideline documents (TGD). Within European chemical and water regimes the TGDs are currently streamlined at European level. This harmonisation of methods is likely to influence both, the other sectors of environmental policy on the European level as well as the existing national risk assessment schemes.
The Federal Environment Agency induced a project comparing the methods under the European REACH-Regulation with national established guidelines for water, soil and the UNECE concept for terrestrial ecosystems. The comparison included the legal frameworks and procedural mechanism for quality assurance. The methodological analysis contained literature work, case studies and interviews with officials to document the experience of authorities and to evaluate the transparency of EQC derivation. The REACH Guidance Documents (GD) served as reference method to identify concordances and differences. Two main procedural "stations"have to be distinguished:
1. Retrieval and Evaluation of all available information [with several "steps"under REACH]
2. Derivation/Identification of the EQS [REACH: PNEC]
As far as the main procedural elements of the first station are concerned a high level of concordances has been identified. However in some respects methodological differences may lead to diverging EQCs:
- Water: The highest level of concordance has been identified between REACH and the European water legislation.
- Soil: The derivation of the EQS differs to some extent since the German approach takes characteristics of the medium soil into account.
- Air: In the field of air quality legislation a case by case approach is dominant basing to a high degree on expert judgement.
Main conceptual differences occur between the REACH-GD and the established concepts in the field of terrestrial ecosystem. In cases where those differences are of minor importance the EQS may be used to fill the gaps in other sectoral legislation, such as provisions for industrial installations (IED 2010/75/EU), water or air quality.

RA11-5
Representativeness of eisenia fetida for the environmental risk assessment of pesticides to soil organisms
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The sole routine testing of the standard earthworm *Eisenia fetida* for the terrestrial risk assessment of pesticides has been under much debate since other soil invertebrates may be more sensitive than this standard test species. Low availability of laboratory toxicity data for taxa other than *E. fetida* has greatly hampered previous sensitivity comparisons. In the present study, the relative tolerance (Trel) approach was applied to enable comparing toxicity thresholds for main terrestrial taxonomic groups and pesticidal types of action (insecticides, fungicides, herbicides, and other) separately. Analyses confirmed previously reported lower and higher sensitivity of collembolans to fungicides and insecticides, respectively. However, various other discrepancies in susceptibility relative to *E. fetida* could be identified using species sensitivity distributions and/or calculated 95% confidence intervals of Trel values. For example, arachnids and isopods were found to be more sensitive to insecticides, and nematodes to fungicides, as compared to *E. fetida*. Implications of study findings for the (first-tier) terrestrial risk assessment of pesticides are discussed.

RA12 - Health and environmental risk assessment of pesticides and biocidal products

RA12-1
Information requirements under the Biocidal Products Regulation and their implications for environmental risk assessment, authorities and applicants
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As of 2013, the current regulatory framework, the Biocidal Product Directive (BPD), is going to be replaced by the Biocidal Products Regulation (BPR). The upcoming regulation will encompass a wide range of regulatory changes. Union-wide authorisation of products, the obligation to substitute active substances with less-hazardous equivalent alternatives, as well as an exposure-based data waiving represent major changes that will affect both authorities and applicants. A further major change concerns the amount of quantitative and qualitative information to be submitted by applicants for both active substances approval and biocidal products authorisation. The BPR requires more compulsory information and exhibits a more extensive list of case-dependent additional information requirements when compared to the BPD. This could represent a major challenge for the applicant, but has to be weighed against the aim to improve hazard and risk assessments in a resource-efficient manner. Current (BPD) and future (BPR) information requirements are compared and discussed and the significance for environmental risk assessments is estimated. In addition, economic implications for applicants are discussed.

RA12-2
Proposal for a harmonized assessment of the mixture ecotoxicity of biocidal products
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Biocidal products are typically mixtures of one or more active substances as well as further ingredients. With the inclusion of the first substances in Annex I of the Biocidal Products Directive (BPD) 98/8/EC the authorisation of the corresponding biocidal products at national level is underway and European Member States (MS) are facing mutual recognitions.
For the authorisation of biocidal products an extensive environmental risk assessment (ERA) is required in accordance with the BPD, i.e. not only every active substance in the product has to be subject of an environmental risk assessment, but also substances of concern, i.e., substances leading to classification of the product or having PBT, endocrine or CMR properties, have to be evaluated separately. In addition estimation of mixture toxicity of the ingredients is required.
As it is well accepted that mixtures of substances usually elicit a different toxicity than the isolated substances itself and additive effects up to synergistic effects are possible, it was agreed between the MS at the Biocides Technical Meeting I / 2011, that the mixture toxicity of the components of biocidal products has to be considered during the ERA and that the concept of Concentration addition is a suitable method for that. However, until now no harmonized concept for the assessment of the mixture toxicity of biocidal products was developed. This means that every MS has its own concept for considering the mixture toxicity during ERA. But this is problematic due to the mutual recognition of authorisations among the Member States.
Therefore the German Federal Environment Agency (Umweltbundesamt, UBA) proposes a tiered approach for the assessment of biocidal products based on the available data for the single product components which also considers the existing approaches of the other MS as well as possible synergistic effects between the product components.
The aim of the approach presented is to harmonize the assessment of the mixture toxicity of complex biocidal products among the MS as well as to assess the mixture ecotoxicity of products and, where relevant, of ecologically relevant mixtures, and at the same time relieve the data requirements for the applicants as well as additional animal experiments.

RA12-3

Prioritisation of biocidal substances for environmental monitoring

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The European Biocidal Product Directive (BPD, 98/8/EC) causes a change of the use of biocidal active substances in EU member states. The placing on the market of a number of substances has already stopped or they will be withdrawn soon as consequence of non-inclusion decisions. Additionally, the use of certain biocides will be restricted by risk mitigation schemes. The expected result of both measures should be a decrease of discharges into the environment of affected biocides. This hypothesis may be proven by an environmental monitoring which might also provide information on the necessity of regulatory improvements (e.g. risk mitigation measures). Therefore, a project was initiated by the Federal Environment Agency of Germany to develop a concept for the selection of biocides for such a monitoring. First, the status of biocide monitoring in Germany was investigated. A questionnaire was sent to authorities involved in routine monitoring as well as to research groups which run projects in this field. Evaluation of about 25 answers revealed that the current monitoring mainly covers surface waters. Often biocidal compounds are monitored due to legal requirements (Water Framework Directive or German Surface Water Ordinance priority substances). However, most of the biocides currently considered are those which are also used as plant protection products. As result of the survey and an additional literature research a database with monitoring data was compiled. Then, a concept was suggested to prioritise biocidal substances for an environmental monitoring. In a first step compounds are evaluated for emission characteristics (mainly based on intended use in BPD product types). The second step covers potential effects. The scores from both steps are combined and used to prioritize compounds. In a third step it is evaluated in which environmental compartment a compound should be investigated (e.g. water, sediment, biota, soil). This evaluation is based on use patterns (product type specific emissions) and substance specific properties relevant for the compartment regarded (e.g. partition between compartments, persistence or BCF). The procedure was tested with a set of 80 biocides which are either already authorised biocides (BPA Annex I) or candidates (biocidal substances currently in the BPA review programme). The plausibility of the prioritisation is discussed with regard to the compiled monitoring data as well as to prioritisation results from other studies.

RA12-4

Pyrethroids: new contaminants in human breast milk

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Pyrethroids are synthesized derivates of pyrethrins, which are natural insecticides that are produced by certain species of chrysanthemum. In the last decades, they have increasingly replaced organochlorine pesticides due to their relatively lower mammalian toxicity, selective insecticide activity and lower environmental persistence. Thus, they are applied in urban area primarily for structural pest control, in agricultural areas on crops, and in the home in pet sprays and shampoos.
Recently some new works point out that its massive use could make pyrethroids considered as pseudopersistent organic pollutant. This means that they may be constantly present in environment not because of its stability, but given that its continuous dumping. Moreover, some studies show that they are toxic, at specific doses on diverse organisms, rats included. As a result of that and as long as World Health Organization marked them as potentially carcinogenic substances, interest for this family compound is increased and some works are come out, mostly about its presence on different kinds of food and natural environment. Nevertheless, studies in breast milk are rarely.
The objective of this work is to study the presence of 12 different pyrethroids in human breast milk samples collected from different areas, including European and South-American countries, with urban and rural areas where different pyrethroids are used. Analytical methodology includes a liquid extraction from freeze-dry samples with an organic solvent and sonication assistant, followed by a SPE cleanup and finally analyzed by GC coupled with MS-MS.
Results indicate the presence of different pyrethroids, with the higher contribution for cypermethrin (with concentration levels up to 16 ng/g lw), and cyhalothrin (up to 8 ng/g dw). Moreover, different pyrethroid distribution between samples was observed comparing different countries. A relationship between total pyrethroids concentration and number of children has been also founded. Pirethroid molecules have different estereoisomers, and that because the isomerspecific enrichment in human breast milk was also studied and checked with environmental data. Finally, and based on the calculated pyrethroid concentrations in human breast milk, the daily ingestion rate (EDI) of each pyrethroid was estimated. The maximum nursing infant dietary intake was 4.60 µg (kg of body weight)-1 day-1 for cypermethrin. This value is lower than ADI (Acceptable Daily Intake) WHO recommends.

RA12-5

New physiology-based pharmacokinetic model for predicting mammalian tissue distribution of pesticides

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Physiology-based pharmacokinetic (PBPK) models are a type of mass-balance model used to predict the concentration profile of chemicals in the blood and tissues of a living animal. PBPK models describe four main processes; absorption, distribution, metabolism and excretion (ADME). Three of the ADME processes are strongly dependent on chemical partitioning properties; absorption, distribution and excretion. A common approximation to describe the partitioning properties involved in these processes is to use a surrogate for storage lipids to estimate the lipophilicity and to assume that the sorption capacity of membrane lipids and proteins is related to the fraction of those phases that has a storage lipid-like sorption capacity. For highly lipophilic, non-polar chemicals the predictions are quite accurate. However, polar chemicals and chemicals with hydrogen bond donors and acceptors can deviate significantly. A more robust method with regard to neutral polar chemicals are poly-parameter linear free energy relationships (PPLFER). In PPLFER equations explicit consideration is given to the different molecular level interactions that may exist between a solute and the solvent molecules of the phase in which it is sorbed; specifically dipole interactions, hydrogen bonding, and van der Waals forces.
An improved PBPK model for predicting total mammalian body burden and tissue distribution of neutral organic chemicals is developed. Partitioning to blood and tissues is built up from their basic as described by appropriate PPLFER equations. The model was calibrated and validated on biomonitoring, occupational exposure and epidemiological studies available in the literature. The model was subsequently applied to a dataset of pesticides with experimentally determined values for the solute descriptors required for application of PPLFER equations. Three different exposure scenarios were considered, corresponding to the three different absorption routes: oral, dermal and inhalation. Overall mammalian body burdens of pesticides resulting from exposure through the three routes of exposure were comparable. However, pesticides with certain combinations of properties have notably different tissue distributions when modelled by the PBPK model based on PPLFER equations.

RA12-6

Evaluation of pesticides in food - A dynamic multicrop model

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Human intake of pesticide residues via food ingestion plays an important role for evaluating current agricultural practice. However, human health impacts of pesticides are still poorly represented in existing assessments, since almost exclusively effects from diffuse emissions are considered, thereby disregarding exposure from residues in field crops after pesticide application. Pesticide uptake and translocation mechanisms vary considerably between crop species and reqire a dynamic assessment.

A new modeling approach was designed to account for pesticide residues in various food crops as source for human pesticide intake. Modeled residues are compared with measured concentrations of 12 different pesticide-crop combinations and correspond well with total crop-specific residual errors ranging between a factor of 1.5 for lettuce and a factor 19 for rice. Intake fractions calculated per unit mass of applied pesticide for 121 substances applied to all crops but potato are usually in the range of 10^{-2} and 10^{-8} kg intake per kg applied for typical times between application and harvest. Intake fractions obtained after direct application were 1 to 5 orders of magnitude higher than intake fractions estimated for indirect emissions, i.e. fractions lost to air and freshwater during application.
Main factors influencing the fate behavior of pesticides are the degradation half-life in plants and on plant surfaces, the residence time in soil as well as the time between pesticide application and harvest. A simplified model based on the most influential input variables enables the prediction of residues within a factor of 10 of those calculated with the complex model. Highest impacts are expected via consumption of herbaceous crops and fruit trees with usually high intake fractions and consumption, while roots and tubers only contribute little due to very low intake fractions. Substitution scenarios enable us to reduce health impacts by choosing alternative pesticides with similar ability to control unwanted pests, but with lower toxicity. However, substitution must be discussed separately within each pesticide target class.

RA14 - Landscape ecotoxicology and spatially explicit risk assessment

RA14-1
Effects of scale on pesticide loss patterns and ecosystem services
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RA14-2
Exposure and ecological risk assessment of herbicides in Japan: validation and factor analysis for predicted concentrations of herbicides by the geo-referenced multimedia environmental model G-CIEMS
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The predicted environmental concentration (PEC) is calculated based on fate models or survey results. Pesticides are characteristically used at limited time points and places, hence for environmental risk assessment it is important to predict temporal-spatial variations of the exposure concentrations. The multimedia environmental fate model G-CIEMS (Grid-Catchment Integrated Multimedia Modeling System) based on Japanese GIS data was developed in the past. In addition, emission estimation methods for herbicides used typically in paddy fields were developed, that were applied to calculate temporal-spatial variations of herbicides concentrations in river waters for the total area of Japan. The model simulations were validated using field survey data from seven rivers. In this study, we focused on the analysis of factors which contribute to the accuracy of model predictions in order to improve the reproducibility of model results. The emission estimation method was divided into following three phases. In the first phase, used amounts of each herbicide formulation, which is the commercially available herbicide product, were predicted for each day for each prefecture. In the second phase, we predicted variations of concentrations for each herbicide in paddy fields and the daily emission ratios to a river and air. In the third phase, we allocated emission amounts of herbicides to GIS segments based on land use data. Finally we calculated environmental concentration for all pesticides for the total area of Japan by the G-CIEMS model. We performed field survey from April 2009 to July 2009 for validation. The maximum concentrations were compared between prediction and observation for the 166 pairs from total 175 pairs (= 7 river sites x 25 herbicides). For compound- or site-related average, more than 70% of the plots had an prediction error of less than one order of magnitude. Based on comparison of several physicochemical properties between higher accuracy herbicide group and lower accuracy one, degradation rate was significantly higher in the lower accuracy group with $p < 0.05$. We confirmed our method have high accuracy for predicting herbicide concentration variations in river for several sites and several herbicides. For improving our method, it is important to investigate actual condition of degradation mechanisms of herbicides in the environment.

RA14-3
Linking exposure and effects of pesticides using passive samplers and the SPEARpesticides bioindicator - a case study in Central Germany, 2010
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Pesticides have always been an important stressor for non-target organisms, and today's modern pesticides are no exemption. Our investigations show the still high impact from pesticides on freshwater communities in selected Central German agricultural landscapes, despite continuous attempts to reduce any unintended effects of the pesticides on the environment.
The study took place in the Bode river catchment located in the TERENO Harz/Central German Lowland Observatory, Central Germany, during the peak pesticide application period in 2010.
At 19 sampling sites along six streams, passive samplers of the type Chemcatcher® were deployed for 2 to 3 weeks to detect any pesticides originating from agricultural field run-off.
For each site, the composition of the aquatic macroinvertebrate community was established and the ratio of pesticide sensitive taxa was calculated according to the bio indicator system SPEARpesticides (SPEAR value; SPEacies At Risk).
The deployed passive samplers detected 16 pesticides in very low concentrations ranging from 0.12 ng to 48.49 ng, proving themselves a reliable tool for the detection of chemicals in surface waters.
Toxic units (TU's) were initially calculated for the obtained time-weighted average pesticide concentrations (TWA) and later re-calculated for realistically estimated pulse exposure time frames of 24 hours and 6 hours, respectively, based on the individual soil organic carbon-water partitioning coefficients (Koc) of all detected substances. The range of TU's shifted from previously -7.7 to -3.4 to now -6.5 to -2.0.
443 Macroinvertebrates belonging to 69 taxa were collected.
The SPEAR values, i. e. the site specific percentages of SPEAR taxa present, ranged from 3.16 to 67.49 (bad < 11 ≤ poor < 22 ≤ moderate < 33 ≤ good < 44 ≤ high).
A significant correlation of the SPEAR values with the respective TU's indicates effects on stream macroinvertebrate communities. Furthermore, the different levels of toxicity towards invertebrates of the different pesticide classes were reflected by their contribution to the site specific TU; herbicides had almost no impact on the macroinvertebrate community whereas fungicides were partially and insecticides mainly responsible for the adverse effects on the macroinvertebrate community.
The re-calculation approach is considered to allow for a more realistic assessment of the dose response relationships (exposure and effects) of pesticides in the fields.

RA14-4
Spatially-explicit exposure and ecological risk modeling tools: SEEM and FISHRAND
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We report on two wildlife exposure models that incorporate the impact of chemical distribution in the environment, habitat suitability relative to areas of contamination, and foraging behaviors of the modeled species. The Spatially Explicit Exposure Model (SEEM) is being developed for the US Army to improve the realism of terrestrial wildlife exposure modeling. SEEM tracks exposures for all individuals in a user-defined population rather than evaluating a single representative individual. Foraging for each individual is guided by habitat suitability preferences. As a result, individuals are less likely to forage in areas where the habitat suitability is low. Also, users may select two different foraging strategies, a free-ranging strategy and a static home range strategy. The model generates population-effects curves. The aquatic model, FISHRAND (FR), is a mechanistic, time-varying bioaccumulation model. The second-order probabilistic model incorporates both sediment and water sources to predict the uptake of organic chemicals based on prey consumption and food web dynamics. The Monte Carlo probabilistic approach allows users to distinguish between sources of uncertainty and variability in predicted fish body burdens. The model allows for more realistic exposure estimates by incorporating data on fish home range, attraction factor (e.g., habitat suitability), and relative abundance. Users can specify preferred habitat areas relative to the contamination profile at the site. Both models offer assessors the tools necessary for advanced exploration of risk drivers and portions of a site in which habitat overlaps with chemical concentrations (and conversely areas where chemicals are present, but habitat is limited).

RA14-5
An agent-based woodpigeon population model used to estimate pesticide exposure in realistic landscapes
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Population modelling is a recommended method to refine risk assessment after the pesticide has failed the first-tier step. We constructed a spatially-explicit agent-based framework (SkyPig) with models of two species: skylark (*Alauda arvensis*) and woodpigeon (*Columba palumbus*) that can be used for population-level assessment of exposure

and effects of pesticides. In our model the birds are characterised by state variables changing dynamically as an effect of their interaction with other agents, environmental resources and time. The common algorithms (mortality check, managing the energy budget, foraging and conducting seasonal activities) operating on these variables result in representation of diverse patterns observed in real ecosystems: population dynamics over the years and foraging patterns including choice of feeding grounds and flocking. These emergent patterns reliably reflect the patterns observed in data describing 40 years long population study in Carlton, Cambridgeshire and radiotracking studies. The distinctive property of our model is the landscape representation: natural structures (like fields or hedgerows) read from GIS maps are implemented as single landscape units without the need for an artificially created grid of hexagonal or square cells.
In this study we present the exposure assessment for a realistic landscape scenario for two fictitious pesticides: pesticide A used as a cereal seed treatment and pesticide B used as a spray applied to oilseed rape. Woodpigeons are known to forage extensively on both cereal grain and oilseed rape leaves and therefore the use of these pesticides potentially exposes them to risk of poisoning. The model predictions on woodpigeon exposure in terms of toxicity-exposure ratios (TER) values obtained by individual birds are compared with TER values calculated for pesticides A and B as used in first-tier exposure model and refined exposure model used in higher tier risk assessment assuming PT and PD values for woodpigeons foraging on sown cereals and oilseed rape leaves.

RA14-6
Accumulation of trace metals in a complex world, validation of a spatially explicit model: BERISP
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Recently, research on accumulation of contaminants to higher organisms has focussed on several environmental factors that may affect food web accumulation. Abiotic factors, species specific traits and habitat have been described to affect accumulation patterns. This implies that spatial variation in environmental factors may play an important role in modulating accumulation. In the current presentation we will present a spatially explicit accumulation model (www.berisp.org), with specific focus on validation of results with field data. The model includes two types of food webs, an omnivorous and an herbivorous one. At the top of the omnivorous food web are two birds species as final receptors: the little owl (Athene noctua) and the blackbird (Turdus merula). Bovine grazer is the consumer in the herbivorous food web. For this study, three field cases were available to validate the models results. For small mammals, data from two case studies are available: the Metaleurop Nord area, near a former Pb and Zn smelter in the North of France, and the Afferdensche en Deetsche Waarden (ADW), a metal-contaminated floodplain in the Netherlands. For the bovine grazers, results from a case study from Hageven, Northern Belgium are used. In that study, two herds of cows were followed in a natural area, and their feeding behaviour was monitored. Preliminary results on small mammals show that in the Metaleurop Nord case the general pattern of the measured concentrations is reflected in the modelled concentrations: shrews> bank vole ~ wood mouse > common vole. The differences between measured and modelled concentrations are not significant for the bank vole. For the wood mouse and shrews, however, the modelled concentrations are higher. For the common vole, this is the other way around. Difference between modelled and measured concentrations are not related to systematic model assumptions, but may be explained by differences in the assumed diet. In the ADW case, modelled concentrations in bank voles and wood mice are similar to the measured concentrations, as is also the case for the beetles. In the presentation, more detailed information on other receptors will be provided, including the effect of inclusion of spatially explicit foraging.

RA15 - Linking exposure to effects in environmental risk assessment

RA15-1
Development of a toxicokinetic/toxicodynamic model for the sublethal endpoint growth of a synchronized Scenedesmus vacuolatus cell population
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Most common ecotoxicological tests assess acute toxic effects by exposing the organism with high dose and short exposure time under laboratory conditions. Process-based toxicokinetic/toxicodynamic (TK/TD) models may be used for extrapolation to chronic toxic effects under field conditions such as fluctuating and pulsed exposures. A TK/TD model simulates the temporal effect course by linking the toxicant exposure concentration to the observable adverse effect via an internal concentration and effect propagation in the organism. Various TK/TD models describe the time course of the endpoint survival of an organism. However, only a few TK/TD models exist which simulate the toxicity time course of sublethal endpoints such as development, growth or reproduction of an organism. The objective of this study was the development of a process-based TK/TD model that describes the sublethal effect on growth of unicellular algae cell populations exposed to toxicants.
We performed a 24 hr algae bioassay with synchronized Scenedesmus vacuolatus cell suspensions which were exposed to six concentrations of Norflurazon, Triclosan and N-Phenyl-2-Naphtylamin, respectively. The endpoints cell volume and cell number were measured in a time resolution of two hours within a one-generation algae cell-cycle.
A model that describes cancer cell growth and the effect of anticancer treatments on cancer cell growth was adopted and modified to the observed growth of Scenedesmus vacuolatus cell population. A cell-cycle kinetic model of the untreated algae cell population was linked to a one-compartment toxicokinetic model. The toxicodynamic model expresses the time-depended dynamics of the affected algae cell growth. Different toxicodynamic compartments represent the effect propagation observable through a cumulative damage with continuous exposure duration. A transition time indicates the propagation duration between two effect levels.
The TK/TD model successfully fitted the averaged algae cell volume exposed to six concentrations of Norflurazon, Triclosan, and N-Phenyl-2-Naphtylamin, respectively. This based on our mechanistic interpretation of algae life-cycle process and toxic effects on algae populations. Moreover, the TK/TD model has the potential to link several effect cascades, such as algae cell growth and algae cell reproduction, within a damage progress. Consequently, chronic toxic effects under field conditions may be simulated.

RA15-2
Putting toxicokinetic-toxicodynamic theory into practice
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Toxicokinetic-toxicodynamic (TKTD) modelling provides applications both for chemical risk assessment and ecotoxicological research. TKTD models quantify the time-course of internal concentration, which is defined by uptake, elimination and biotransformation (TK), and the processes which lead to the toxic effects (TD). We present three different applications of TKTD modelling: 1) modelling survival in multiple pulse exposures, where we tested the calibration data requirements and model assumptions, 2) studying the mode of toxic action of pesticides and 3) explaining differences in sensitivity between species. We calibrated TKTD models for *Gammarus pulex* and *Gammarus fossarum*, exposed to pesticides diazinon, imidacloprid and propiconazole. To calibrate the models, we conducted toxicokinetic experiments (internal and external concentrations measured), acute toxicity experiments (4-d standard LC50 tests) and pulsed toxicity experiments (1-d exposure pulses). 1) We simulated survival of *G. pulex* in pulsed exposure to propiconazole using a TKTD model calibrated with acute toxicity data and compared the prediction with experimental results. The comparison showed that the model overestimated mortality in pulsed scenarios, which suggests that acute toxicity data could be used to calibrate TKTD models to achieve protective predictions in pulsed exposure profiles. To assess the need of TK in survival models, we included or excluded simulated internal concentrations based on pre-calibrated TK. The differences between goodness of fits of the models including or excluding TK were small. 2) To investigate whether propiconazole is acting specifically or as a baseline toxicant in *G. pulex*, we compared internal propiconazole concentrations in *G. pulex* during toxicity tests with internal lethal concentrations (ILC50) of known baseline toxicants in *Daphnia magna*. The internal concentrations of *G. pulex* reached the ILC50 range of baseline toxicants in *D. magna*, which indicates that propiconazole acts as a baseline toxicant during 10-day exposure for the endpoint survival. 3) We observed that *G. pulex* is more sensitive to diazinon than *G.fossarum*. Diazinon is an acetylcholinesterase (AChE) inhibitor and it requires metabolic transformation to diazoxon to inhibit AChE efficiently. When we compare the TKTD parameter estimates of *G. pulex* and *G.fossarum*, we see that the elimination of diazoxon from *G. pulex* is much slower, which might explain its higher sensitivity to diazinon.

RA15-3
Chronic effects on pairing behaviour and reproduction of Hyalella azteca following pulse exposure to permethrin
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Exposure of non-target aquatic organisms to pesticides often occurs in short pulses following periods of drain flow, surface run-off or spray drift. Both acute and chronic laboratory studies use maintained exposures whereas in the field time varying exposures are likely to occur, with the potential to cause both acute and sub-lethal effects. There is therefore a mismatch between laboratory and field exposure patterns.
The aim of the present study was to examine short-term and long-term effects of 1 hour pulse exposure of different concentrations of the pyrethroid pesticide, permethrin, on precopulatory pairs of Hyalella azteca and to determine the effect on pairing behaviour and subsequent reproduction over an 8 week period after exposure.
Before molting, pairs of H. azteca swim together in amplexus where the adult male grasps the female with its gnathopods. Swimming in amplexus plays a key role in the reproductive cycle and is therefore essential for successful reproduction in H. azteca. Very little is known concerning the effect of pesticides on pairing behaviour and subsequent reproduction of H. azteca.

Pairs of H. azteca were pulse exposed to a single pulse of 1 hour to different nominal concentrations of permethrin; 0, 0.3, 0.9 and 2.7 µg/L. After exposure the pairs were transferred to clean water. During an 8 week test period the treatments were monitored for pairing behaviour and every second week the offspring were counted.
Pulse exposure of pairs to permethrin affected the time to reform pairs. Pairs exposed to 0.9 and 2.7 µg/L took longer to re-form compared to controls and pairs exposed to 0.3 µg/L. Furthermore the average reproductive output of H. azteca was lower for pairs exposed to 0.9 and 2.7 µg/L during the 8 week test period compared to the control groups.

RA15-4

The relevance of toxicokinetic-toxicodynamic processes for the population recovery of Gammarus pulex after exposure to pesticides

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Exposure to pesticides can lead to adverse effects on their survival, the magnitude of which depends on pesticide fate in the environment and the intrinsic sensitivity of exposed organisms. Standard ecotoxicological practices calculate the magnitude of these effects based on maintained exposure concentrations using dose-response models. However, in the field exposure patterns are often more complex. In order to take account of such exposure patterns, an approach that includes toxicokinetic (uptake and elimination) and toxicodynamic (internal damage and recovery), TK-TD, can be used to describe processes within exposed organisms. Recovery of populations from adverse effects is used as a proxy for acceptability of some adverse effects on non-target populations. The potential for population recovery depends toxicant, species specific factors and habitat structure and timing of pesticide applications.
Here we explore the joint impact of intrinsic sensitivity and pesticide specific factors on the population recovery. We developed an individual-based model (IBM) to simulate the response and the subsequent recovery of amphipod populations exposed to four pesticides in different exposure scenarios. Pesticide induced mortality was implemented with two different models. Toxicokinetic-toxicodynamic processes were accounted for by implementing the threshold damage model for survival in half of the treated populations. For the other half, we used a logistic dose-response model. Simulated populations were exposed to 24h, 96h and 16 day LC50 of diazinon, chlorpyrifos, carbaryl and pentachlorophenol on May 1st in the simulated year. Population recovery was compared in populations where we accounted for TK-TD processes, hereafter termed TDM-populations, and those where we used a dose-response model for survival, termed DR-populations.
Calculations of the mortality rate in populations exposed to chlorpyrifos, resulted in much more severe mortality in TDM-populations, when compared to DR-populations. These differences resulted in substantial differences in population recovery times. Recovery after 16 day exposure to LC50 of diazinon took the longest, followed by recoveries after chlorpyrifos, carbaryl and pentachlorophenol.
In conclusion, accounting for toxicokinetic-toxicodynamic processes results in differences, based on different pesticide characteristics, in magnitude of mortality and subsequent recovery times and yielded, on average, longer recovery periods.

RA15-5

Linking pesticide exposure to spatial dynamics: an individual-based model of wood mouse populations

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In pesticide risk assessment, risk is defined as a result of hazard and exposure. The less time animals spend in treated fields the less they will be exposed to pesticides and the risk is thus lower. Therefore, the spatial and temporal distribution and behaviour of non-target species are important in risk assessment. We studied the relationship between the spatial and temporal dynamics and the level of exposure by constructing a spatially explicit individual-based population model, using wood mice (*Apodemus sylvaticus*) on arable fields typical of the UK as an example. The model was constructed based on literature data on wood mouse life-history traits and behaviour. To capture the presence or absence of wood mice in certain fields on certain days, nesting and foraging behaviour and the corresponding movements were represented phenomenologically. Additionally, crop rotation and farming practices affecting the wood mice's behaviour were included. The model is designed to link pesticide exposure and farming practices to the spatial movements and location of individual mice to study the effects of exposure at the population level. We briefly describe the model and then use two example scenarios to demonstrate the potential use of the model for ecological risk assessment of pesticides, addressing the question: how is the (i) spatial and (ii) temporal distribution of the mice, depending on crop type and season, related to pesticide exposure?

RA16 - Monitoring data and post-registration studies: generation, compilation and use in the environmental risk assessment and management

RA16-1

Pre and post-authorisation monitoring for pesticides focussing on birds and mammals - recent developments from the SETAC environmental monitoring action group (EMAG)

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Bird and mammal risk assessments for individual pesticides carried out under EU Regulation 1107/2009 routinely use the relevant guidance document issued by EFSA (EFSA, 2009)1. This guidance outlines procedures of toxicity and exposure assessments for lower tiers. If concern is raised regarding lower tier assessments it may be possible to refine the risk assessment and although a range of options are available, detailed guidance is lacking as regards how to proceed. One possible refinement mentioned in EFSA (2009) is the use of field studies where 'field studies' refers both to studies of effects following experimental pesticide applications (i.e. applications made as part of a regulatory study) and also to 'active monitoring' of effects following applications of authorised products in agricultural practice. EFSA (2009) also highlights the potential usefulness of 'passive' wildlife incident monitoring or surveillance, involving investigation of suspected incidents reported by farmers and members of the public. The Environmental Monitoring Action Group for Pesticides (EMAG-PEST) of SETAC has been investigating the range of both pre and post-authorisation studies that have been conducted as well as the experience gained, with a view to consolidating 'best practice'.

RA16-2

Post-authorisation monitoring for mammals, birds and insects - wildlife incident investigation scheme - England

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The Wildlife Incident Investigation Scheme (WIIS) is a reactive surveillance scheme that monitors the suspected pesticide poisoning of wild animals, companion animals (pets) and beneficial insects. The suspected pesticides include plant protection products and biocides used to control vertebrate pests and similar schemes operate in England, Wales, Scotland and Northern Ireland. WIIS is partly funded by a levy on pesticide sales in the UK and it is co-ordinated by the Chemicals Regulation Directorate of the Health and Safety Executive (HSE), which is the lead authority on pesticide legislation. It has operated within a legal framework since the Control of Pesticides Regulations (COPR) 1986 and given this longevity and funding arrangements, it is probably unique in the world. The results from WIIS form part of the pesticide regulatory process and are reported quarterly on the internet. The majority of poisonings involve the intentional, illegal use of pesticides and where there is an infringement of legislation on pesticides or the environment, appropriate enforcement action may be taken by the Police, HSE or the local authority. How WIIS operates and the results of investigations into suspected poisonings in England will be discussed. This will focus on investigations where pesticides are used for their intended purpose. For example, honeybee poisonings from spray applications or feral bee treatments and slug pellet applications and rodent control for incidents with mammals and birds. The extent and possible reasons for the intentional, illegal use of pesticides will also be highlighted. Due to improved analytical methods that were introduced in 2010 (unpublished), WIIS has reported an increase in the number of bee incidents where multiple pesticides and/or very small pesticide residues have been confirmed. It is unlikely that these were the cause of death of the bees, but pesticides found include thiacloprid, dieldrin, chlorpyrifos, fipronil and propiconazole. The agricultural use of pesticides may not be involved in some of these incidents and hive wood treatments, amateur garden uses, or pet animal treatments are suspected. An effective, comprehensive and consistent approach to a monitoring scheme is an expensive commitment and a collaborative project among the major disease and contaminant monitoring schemes in the United Kingdom is now facilitated by the Wildlife Disease & Contaminant Monitoring and Surveillance WILDCOMS Network.

RA16-3

Bee health in Europe - facts & figures, A OPERA document

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Declines of managed honey bee colonies and also of some wild bee species have been reported by many countries, leading to intensive work and actions in the areas of research and regulations. Declines in pollinating insect numbers can have significant adverse effects ecologically on the diversity of plant species and economically in the productivity of crops. However, up until now, the status and relative importance of the stress factors that may affect bee populations have been relatively unclear and, in many instances, widely disputed.

In this context, OPERA, has undertaken to produce an updated review on the issue of honey bees and pollinators in Europe, with some highlights to other continents, which would cover ecological and economical aspects related to these species in relation to agriculture.

The expert invited have gathered the latest information available on the factors influencing the health of both managed honeybees and populations of native wild bees, including solitary bees and bumble bees. The main conclusions indicate that the honey bee can cohabitate with modern agricultural practices provided necessary precautions are taken to maintain viable food resources for bees and avoiding practices that may cause adverse effects. These precautions include the design of agricultural landscapes and the implementation of practices that account for the presence of pollinators. Essential developments also concern the availability of effective and regulated veterinary compounds to help beekeepers eradicate the most important pests from apiaries. An analysis of beekeeping activity in its economical context is also provided. Finally, modern agriculture and beekeeping demands better technical knowledge and a critical lack of training and communication to better accompany the updates in science and technology to the farm and the field is identified.

The case of wild bees may be considered to be very similar to that of the domesticated honey bee albeit far less well documented.

Recommendations are emitted towards all those involved in agriculture, bee keeping regulatory authorities and research, which should be communicated to all as the effectiveness of the actions will rely on their common effort to implement them.

RA16-4

Contamination of flowering crops by insecticidal dust drift - effects on honey bees (Apis mellifera L.)

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In 2008 a large-scale honey bee poisoning in parts of southern Germany occurred during sowing of maize. This incident was caused by contamination of flowering bee forage plants with drift of dust from the insecticidal seed-dressing containing the active substance Clothianidin.

Since early 2009, practical and large-scale drift experiments during sowing insecticide treated seeds were realized to investigate the link between abrasion potential of treated maize and oilseed rape seeds (determined by Heubach values), dust drift and resulting residues in adjacent flowering crops as well as the effects on honey bees. In 'worst case' scenario experiments bee colonies were set up in semi-field and field trials along the edges of the drilled area (treatment) to study the impacts of dust drift on mortality, foraging activity and brood development in bee colonies (exposure to dust during sowing and contaminated pollen and nectar) using drift-reduced pneumatic sowing techniques. Drilling was conducted during bee flight activity, so foragers were continuously exposed to dust. Two control variants were set up with hives in about 50 m (control) and more than 500 m (remote) distance to the exposed forage plants.

No adverse effect on bees and bee colonies were detected after rape sowing in 2009 and 2011. However, during maize sowing in 2010 and 2011 bee mortality was clearly increased.

Semi-field experiments with manual application of insecticide-loaded maize dust in Phacelia (Phacelia tanacetifolia Benth.) were carried out to analyse the impact of different rates of the active ingredient (0.5 g a.i. / ha and 2.0 g a.i. / ha Clothianidin) and different particle sizes ($x \leq 160$ µm, $250 < x \leq 450$ µm, $x > 500$ µm) of dust on mortality, foraging activity and brood development in bee colonies.

In contrast to the other dust fractions, at the same rate of Clothianidin for fine dust particles '$x \leq 160$ µm' significant mortality was detected. Studies on different rates showed effects on mortality only for the higher rate, whereas no differences were detected between the low rate and the untreated control.

Despite improvements in seed dressing quality and development of drift-reducing sowing technique since 2008, there is a continuous need for further improvements to exclude adverse effects on bees, especially for maize seeds.

Acknowledgement: The work was financed through the Diabrotica research program funded by the Federal Ministry of Food, Agriculture and Consumer Protection (BMELV).

RA16-5

Exposure of soil organisms to plant protection products - Monitoring the vertical niche differentiation of soil microarthropods in an arable field in the course of a year

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According to the new pesticide regulation 1107/2009 the necessity to conduct soil macro-organism studies is triggered by the mode of application and the impact of substances on NTA rather than by the DT90. As a consequence the need to test springtails and mites in lab and field studies is increasing. Additionally more attention is drawn on the ecology of soil microarthropods. A crucial point under discussion is the exposure of soil fauna. Recently published "EFSA opinions"pointing at the fate of pesticides in the soil compartment, the relevance of the soil litter layer and the soil ecoregion concept take this feature particularly into account. As a result it is assumed, that the "worst case soil depth profile for short term risk assessment would be litter (if present) or 0-1 cm depth instead of the currently used 0-5 cm depth"(EFSA 2010). With our recent results we complete the dataset presented at the last SETAC Europe meeting in Milano 2010 (Theißen et al. 2010) to increase knowledge on the spatio-temporal dynamics of microarthropod-assemblages in the topsoil of arable fields. Within one year soil cores (5 cm in diameter; 10 cm in depth) were taken monthly, divided into four layers (0-1 cm, 1-3 cm and 3-5 cm and 5-10 cm respectively) and extracted for Collembola, Oribatida and Mesostigmata by means of heat extraction in a Macfadyen apparatus. The results contribute to a sound development and evaluation of exposure scenarios compared to effect thresholds obtained in standardised ETX-tests. EFSA Panel on Plant Protection Products and their Residues (PPR) (2010): Scientific Opinion on the development of a soil ecoregions concept using distribution data on invertebrates. EFSA Journal; 8(10):1820. [77 pp.] Theißen, B., Larnaudie Lopez, M.I., Michala, M., Leicher, T.: Spatial and temporal distribution of soil microarthropods in in-crop habitats. Poster SETAC Europe 21st Annual meeting 15.- 19. May 2011, Milano, Italy.

RA16-6

Use of groundwater monitoring data for existing agrochemicals to support re-registration

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In order to fulfil regulatory requirements for agrochemicals in the EU, the predicted environmental concentrations in groundwater (PEC_{GW}) are estimated using FOCUS models. Depending upon the uses to be registered, up to nine groundwater scenarios are modelled. The resulting concentrations are compared to a non-health-based cut-off criterion of 0.1 µg/litre. This modelling is designed to be conservative and thus tends to overestimate the concentrations in even the shallowest aquifer. Recent revisions to the criteria governing the selection of modelling endpoints, such as the FOCUS Kinetics guidance, have tended to increase the conservative nature of the modelled PEC_{GW}.

As increasing numbers of agrochemicals will not pass this arbitrary assessment step in the future, it is necessary to develop acceptable higher tier methodologies to refine the modelled output using real-life retrospective groundwater monitoring data. Data from a number of such studies with the maize herbicide, terbuthylazine, will be described and the potential acceptability of such data sets for the regulatory process will be discussed with special reference to key criteria that must be met for the data to be considered sufficiently robust to be used. Implications of the application of groundwater monitoring study data as a higher tier of assessment will be discussed.

RA17 - Multiple stressors in a changing world

RA17A-1

A close look at the temperature-dependent chemical toxicity to aquatic organisms and its implication on derivation of water quality guidelines for protecting aquatic life

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The anticipated anthropogenically-driven climate change not only can increase the average air and water temperatures and prolong the hottest period, but also result in

increased incidents of temperature extremes that will have profound implications on the toxicity of chemical contaminants and hence their ecological risks to aquatic organisms. In this talk, I will comprehensively examine and discuss the mechanisms of temperature-dependent chemical toxicities to aquatic ectotherms based on both literature review and empirical laboratory studies. Examples will be drawn from an array of marine organisms including amphipod, copepod, diatom, and fish after exposure to a chemical (e.g., chlorothalonil, copper, copper pyrithione, DDT or nano-zinc oxide (nZnO)). In general, we observed that chemical toxicity often increases with increasing temperature over the thermal tolerance range (TTR) of a species, and is further exacerbated at extreme temperatures (i.e., lower or higher than the TTR). Most of the aquatic organisms showed the highest tolerance to chemicals at their optimal temperature(s) where they displayed the highest value of median lethal or effect concentration. For aquatic animals, such universal phenomena can be well explained by the oxygen limited thermal tolerance theory established by Hans Pörtner. Moreover, the overall temperature-dependent toxicity profiles vary considerably amongst different chemicals. Such differences may be partially attributable to the differences in temperature-mediated modifications of their physicochemical properties, toxicokinetics and bioavailability. For instance, we observed that ion dissolution of nZnO in seawater significantly increases with decreasing water temperatures. The diatoms exposed to nZnO had a significantly reduced growth rate at the lowest experimental temperature in contrast to the control; this response was probably due to the increased availability of toxic Zn ions at low temperatures. Recently, we have been conducting a novel meta-analysis to address whether an assessment factor of 10 (AF10) applied to fresh water quality guidelines (WQGs) would be sufficient to account for variation in chemical toxicity brought by thermal extremes. Our preliminary results suggest that AF10 seems adequately protective. Implications of our results will be discussed in relation to ecological risk assessments of chemical contaminants and derivation of WQGs for protecting aquatic life.

RA17A-2

The calculation of risks due to mercury and other stressors to multiple endpoints at a regional scale for the South River and Upper Shenandoah River, Virginia USA.

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A cumulative integrated risk assessment has been performed for the South River from the area upstream of Waynesboro VA to the uppermost part of the Shenandoah River. The area is a site of historic mercury contamination from synthetic fiber production in Waynesboro. Six risk regions have been delineated. Other sources of other stressors include urban and agricultural run-of, channelization, erosion, and contaminated sediments and biota. The current iteration of the relative risk model (RRM) incorporating the hierarchical patch dynamics paradigm was used to construct a conceptual model, designate risk regions, create a ranking system and calculating risks to the stakeholder derived endpoints and impacts. In concert with this effort a Bayesian network was constructed using the same risk regions, sources, stressors, habitats and impacts. The use of the Bayesian network allows a straightforward calculation of management requirements to reduce risk in each of the six risk regions. Atypically, the current source of the Hg contamination is the environment itself. The warm water fish species have been found to have consistently high tissue concentrations downstream of the original source. Temperature may also be a risk factor affecting fish reproduction. Nutrients from upstream of Waynesboro also may be contributing to risk to a variety of endpoints. Although intensively studied for a number of years, the lack of data from upstream and from within the watershed are contributing to the uncertainties in the risk estimates. Our results demonstrate that the risk is unevenly distributed along the course of the river. Mercury is the stressor contributing the highest risk but other stressors are large contributors. The endpoints at highest risk are those directly associated with ecological services. The Bayesian networks excelled at examining risks to specific endpoints while the RRM demonstrated relationships between endpoints. This research program identifies risks and demonstrates the benefits of an integrated risk, research and management program in the restoration of watersheds at a regional scale.

RA17A-3

Application of toxicological and ecological concepts to analyse multiple stress in aquatic communities

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As a result of the increasing human impact on aquatic ecosystems, freshwater organisms are often exposed to multiple stressors simultaneously, which can result in combined effects, leading to serious consequences for ecosystems. There is a clear need to develop a better understanding of interactive effects on ecosystems. Therefore, already existing concepts and tools in ecotoxicology and ecology have to be proofed for their validity and applicability in complex community responses to multiple stress.
A microcosm study was conducted under controlled conditions and periphyton was used as test community. The effects of a resource stressor (elevated conductivity) and a toxic stressor (prometryn) were analysed independently and both in combination. Effects were compared to untreated controls. Structural (biomass, algal class and diatom composition, and functional parameters (tolerance development) were determined over a growth period of 6 weeks.
Ionic stress clearly influenced structural properties of communities, whereas prometryn as single and combined toxic stressor led to functional and structural changes of communities. Diatom compositions clearly respond to different treatments, representing *Navicula halophila* as salt tolerant species and *Fragilaria capucina* as tolerant to toxic stress. Both stressors in combination lead to a completely new community structure with high abundances of omnipresent diatom species. Functional changes of the community were quantified by PICT (pollution-induced community tolerance). The exposure to prometryn increased the tolerance of all exposed communities, independently from the ionic load of the treatments. According to the EC_{50} of P5000, high ionic loads (5000 µS cm^{-1}) and prometryn showed a synergistic interaction because their combined effect was clearly larger than the predicted EC_{50} (calculated by the model of independent action, based on the individual single effects).

RA17A-4

Responses of mean species traits in communities to multiple environmental stressors and the ecological risk assessment based on ecosystem function

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A trait-based analysis was conducted on a long-term (25 years) monitoring data of zooplankton community of Lake Kasumigaura, to elucidate relative importance of environmental stressor (temperature changes, nutrient loadings, and chemical pollution) for the temporal changes in zooplankton community with respect to their contribution to an ecosystem function. I used the trophic transfer efficiency across three trophic levels as a measure of ecosystem function. Based on this measure, I identified species traits that were important for this function with a simple ecosystem model (the conversion efficiency of zooplankton was one of the most important traits). For the trait-based analysis, I made a database of traits (e.g. conversion efficiency, optimal temperature, range of suitable temperature, saprobic index, tolerance to chemical [carbaryl acute toxicity], median food size, and body mass) for major zooplankton species in Lake Kasumigaura. The long-term temporal changes of biomass-weighted mean traits in two seasons (summer: May-September, and winter: October-April) were separately analyzed in conjunction with the environmental factors. The water temperature has been increasing at approximately 0.027 oC per year (climatic warming). There were long-term trends in traits: the mean body size and the mean tolerance to chemical had peaks on early 1990s but are decreasing in summer. In winter, however, they are increasing in recent two decades. The conversion efficiency is also increasing in summer but decreasing in winter. These observations suggest that the ecosystem function is severely deteriorated in winter. Similarities of temporal patterns between the functional traits and the environmental factors were examined with the Wavelet analysis. The results indicated that the zooplankton community synchronized clearly with water temperature in both seasons. The effect of inflated temperature was positive for the conversion efficiency in summer although this effect would be conditional of reduced chemical pollution because the tolerance to chemical was highly correlated with the temperature preference of zooplankton.

RA17A-5

Discriminating the effects of pesticide stress and habitat degradation on stream benthic invertebrates

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Achieving a good ecological status for waterbodies requires the identification of the relevant stressors to implement adequate measures. While the reduction of organic load resulted in acceptable low levels, restoration of the natural river morphology is now believed to be the most urgent task for water managers. Yet, several of these measures failed to rehabilitate the expected near-natural communities. At the same time, pesticides are frequently detected in surface waters that may limit the recolonisation of sensitive invertebrate species. The aim of the present study was therefore to discriminate between the effects of morphological degradation and pesticide stress on invertebrate communities. For this purpose, the $SPEAR[\%]_{habitat}$ index was introduced to identify the effects of habitat loss due to morphological degradation, which was not intercorrelated to the other metrics. To quantify habitat loss, relevant in-stream variables available from field surveys were identified by PCA and combined to an overall habitat degradation score (HDS) for multiple regression modelling. To quantify pesticide input, the established run-off potential (RP) model was applied. Many of the classical metrics, such as the EPT Index or the German Fauna Index were highly interrelated and identified the predominant alkalinity gradient as major stressor. This was also the case for the SPEAR[%] index, which was expected to solely indicate pesticide stress. However, also the RP and the number of recolonization stretches (RS) were included in the best fit model of this metric, which had the overall best correlation of biological indices and environmental variables. The $SPEAR[\%]_{habitat}$ was not intercorrelated to the other metrics and identified the MDS as most important variable, although the correlation was not as strong as others. This correlation was even stronger for sites with low potential pesticide pollution, as indicated by high SPEAR[%] values and a low percentage of agriculture in the catchment. Our results suggest that pesticide stress has a similar or even higher impact on the ecological status than morphological degradation and that current-use degradation metrics are also influenced by pesticide stress. The latter may have important implications on future assessments of ecological status. Finally, the presence of recolonization stretches upstream alleviated the effects of pesticides in terms of higher SPEAR values, which could be used as potential management option.

RA17A-6

Ranking the impacts of multiple environmental stressors on freshwater invertebrate and fish communities

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Community composition and structure are largely determined by environmental stressors which have selected species able to survive, grow and reproduce under given conditions. Human activities like habitat degradation or toxicant release represent additional stressors potentially modifying the selection processes and affecting biological communities. Understanding those filtering mechanisms and disentangling the impacts of multiple stressors is vital to underpin management measures to avoid or reduce biological impairment. The goal of this study was to disentangle the individual influences of 20 natural and non-natural stressors pertaining to four categories (geography, physical habitat quality, water chemistry and toxic pressure) on eight endpoints summarizing freshwater fish and invertebrate communities. Toxic pressure was expressed for five groups of chemicals as the multi-substances Potentially Affected Fraction (msPAF) of species, derived from species sensitivity distributions (SSDs). We used a relatively new, non-parametric modelling technique, Boosted Regression Trees (BRT), to separate and assess individual stressors' impacts and visualize data-driven response curves. The models behaved well in terms of predictive power, with an explained variance above 60% for five out of eight endpoints. Overall ranking was relatively similar among the different endpoints, with recurrent predictors including geography (especially drainage area and latitude/longitude), physical habitat quality and water chemistry variables (particularly the phosphorus concentration, pH and total Kjeldahl nitrogen). The five toxicant groups together explained between 5.2 and 17.4% of the total variance in the biotic endpoints, and specific patterns of response were observed for endpoints related to sensitive taxa or physiological impairment. Partial dependency plots, free from distributional assumptions, provided insight into the direction, shape and thresholds of single predictor-response relationships. Boosted Regression Trees proved an appropriate approach to investigate the individual impacts of combined stressors on species assemblages in the field.

RA17B-1
The importance of seasonal resolution to modelling the interaction of bioaccumulation and climate change
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From 16-21 July, 2011 a SETAC Pellston workshop was convened to assess the influence of global climate change (GCC) on the scientific foundation and practice of environmental toxicology and chemistry. Workgroup 1 focused on influences on chemical occurrence, fate and bioavailability. Here, I present our results for GCC impacts on bioaccumulation. These impacts occur through three primary mechanisms: influences on environmental exposure, on dietary exposure and on within-organism uptake and loss rates driven by bioenergetic processes. This work focuses on the bioenergetic-mediated impacts of GCC, building on previous modeling of species in the Laurentian Great Lakes.
A bioenergetics model for round goby (Apollonia melanostomus) was parameterized to reflect growth rates observed in Lake Erie, Laurentian Great Lakes. The impacts of climate change on bioenergetics was assessed based on a shift towards warmer annual lake surface temperatures. Simulations were run for the baseline case and for a 1, 2, and 3-degree Celsius increased annual average temperature. The effects of this warming on chemical bioaccumulation were then estimated by coupling the bioenergetics model to a mechanistic bioaccumulation model for a broad range of hypothetical chemicals with log octanol-water partition coefficients (KOW) ranging from 0 to 8 and biotransformation half-lives ranging from 0.1 to 1000 days.
The impact of GCC on round goby growth illustrated the non-linear interaction between growth rate and fish thermal range. Two scenarios were chosen to showcase the impacts of GCC on bioaccumulation: the highest growth scenario, and the warmest scenario. When only annual average concentrations were considered, little difference among scenarios was evident. However, when the seasonal patterns of bioaccumulation were considered, substantial changes, both increasing and decreasing bioaccumulation, emerged. These seasonal impacts, which were more pronounced for metabolizable chemicals than for persistent ones, could be particularly important when they intersect with other time points, such as commercial fishing seasons or critical life stages for toxicological impact. The magnitude of the deviation from the baseline case depends most strongly on the biotransformation half-life, and then on KOW.

RA17B-2
Additive pressures from herbicides and elevated sea surface temperatures on symbiont-bearing foraminifera from the Great Barrier Reef
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Coral reefs are threatened globally by the combined effects of climate change and decreased water quality, especially in the tropics where monsoonal rainfall can deliver vast amounts of terrestrial contaminants to inshore reef systems. It has been hypothesized that reducing pollution could increase resilience of tropical ecosystems to climate change but empirical support for this strategy is extremely limited. Our research focuses on how temperature thresholds of symbiont-bearing species are impacted by different water quality scenarios. Both herbicides and elevated temperatures have been shown to disrupt the relationship of reef building invertebrates with their microalgal symbionts and as both factors potentially interfere with photosynthetic electron flow, additive or interactive effects may occur. In a series of laboratory studies, we examined the potential of stress caused by low concentrations of the photosystem II (PSII) inhibiting herbicide diuron on several types of symbiotic algae (diatom, dinoflagellate or rhodophyte) within the tissues of benthic foraminifera from the Great Barrier Reef. Symbionts within foraminifera were always more sensitive to thermal stress in the presence of diuron (≥ 1 µg L^{-1}). Diuron had a direct effect on photosynthetic efficiency (reduced effective PSII yield $\Delta F/F'm$), while elevated temperatures (> 30°C, only 2°C above current average summer temperatures) were observed to impact photosynthesis indirectly by causing reductions in maximum PSII yield (Fv/Fm), interpreted as photodamage. The mixture toxicity model of independent action revealed response additive combined effects of temperature and diuron for inhibition of photosynthesis and the onset of photodamage. Additionally, combinations of diuron and elevated temperatures were shown to cause bleaching through loss of chlorophyll a in foraminifera hosting either diatoms or dinoflagellates. We thus demonstrate that locally improving water quality can enhance resilience of symbiotic phototrophs to global stressors such as projected increases in ocean temperatures.

RA17B-3
How climate change scenarios will affect toxicity: assessing multiple stressors using a Heliocidaris tuberculata sperm bioassay
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Marine ecosystems are facing dramatic changes as a result of climate change. Changes in the physicochemical parameters of seawater systems, as a result of climate change, can potentially alter a number of factors that determine toxicity for any given pollutant. For marine systems, it is accepted that the world will contain warmer, more acidic oceans under future climate change conditions. These changes alone (increased temperature and/or decreased pH) have been shown to influence survival, development and reproduction for many marine species. However, such effects have always been in uncontaminated waters. The reality is that many marine species will face the effects of changes in seawater physicochemistry in combination with toxicant stress.
In order to better understand the combined effects of copper, elevated temperature and lowered pH on fertilisation success of an endemic Australian sea urchin, *Heliocidaris tuberculata*, we present a study incorporating multiple stressors (3 temperatures x 3 pH x presence/absence of copper). The nominal copper concentration applied in these tests was based upon an EC_{50} calculated from five standardised toxicity bioassays. Potentiometric titration was performed to ensure pCO_2 levels were maintained at conditions expected for eastern Australian coastal waters for the end of 2100 scenarios.
Results show that temperature and copper had a synergistic impact upon fertilisation, significantly ($p < 0.05$) reducing fertilisation success by > 50%. With temperature alone also being a significant factor ($p < 0.001$), we suggest that exceptional future warming of eastern Australian coastline waters may limit the spawning season of *H. tuberculata*, which is already sensitive to high summer temperatures. Acidification, as a sole stressor, showed no significant effect on fertilisation (p=0.098). However, in combination with copper, low pH caused a significant decline in *H. tuberculata* fertilisation success ($p < 0.001$). As found in other studies, we conclude that sea urchin fertilisation may be robust to changes in pCO_2 under clean water conditions, but that in combination with other stressors, such as temperature and/or pollution, changes in ocean physico-chemistry may pose a risk to continued recruitment. This study particularly highlights the importance of addressing the potential for interactive effects between climate change stressors and common marine pollutants.

RA17B-4
Evaluation of the combined action of natural stressors and chemical pollutants in algae. Assessment of functional, structural and metabolism alteration
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Nowadays, there is a growing number of studies exploring the combined effect of different stressors on ecosystems. However, the interactions between natural stressors and toxicants are still poorly understood. Among the stressors that might influence ecosystems, toxicants can directly or indirectly affect all relevant ecosystem processes such as primary production. On the other hand, fast and intense changes in the water temperature is one of the major threats for freshwater ecosystems.
The objective of this study was to characterize the physiological responses of cultured algae, Scenedesmus vacuolatus in response to physical (temperature) and chemical (anthropogenic contaminants) stressors. The pollutans selected for this study were the priority pollutant diuron (herbicide, PSII inhibitor) and the emerging compounds propranolol (Î²-blocker) and fluoxetine (antidepressant).
The experiment followed a factorial design with 2 factors (water temperature and toxicant concentration) and their interaction. A previous experiment determined that the optimal temperature was 20Â°C, while 30Â°C was used for simulating physical stress. Chemical stress was reproduced at the level of EC30 for each toxicant (5, 850 and 500 Î¼g/L for diuron, propranolol and fluoxetine, respectively). Changes in photosynthetic efficiency (Yeff), photosynthetic capacity (Ymax), photochemical quenching (qP) and non photochemical quenching (NPQ) were studied in control and exposed algal cultures.
The algal toxicity of the three compounds differed considerably. Diuron was the most toxic compound, followed by fluoxetine and propranolol. Effects of diuron occurred

immediately after addition, which indicates a very specific toxic action of this compound to algae (inhibition of photosynthesis). Propanolol and fluoxetine toxicity effects appeared later than those detected with diuron exposure (after 30 minutes). Most of the endpoints were affected after 12 hours for all the compounds tested, except in the case of diuron, where NPQ mechanisms were inhibited after 12 hours of exposure, suggesting damage in the pigments where the NPQ takes place.
The increase of temperature reduced the toxic effect of the herbicide diuron and propanolol at the beginning of the exposure as well as at the final time. In the case of fluoxetine, the temperature increase reduced the toxicity at the initial time, but a synergistic effect was observed at final time with an enhanced toxicity.

RA17B-5
Chemical exposure enhances outbreak of infectious disease in fish
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Heavy oil (HO) pollution is one of the most important environmental issues in the world. In our previous study, we evaluated immunotoxic effects of HO on Japanese flounder Paralichthys olivaceus, and found that 0.3 g/L of HO led immune suppression at cellular and molecular levels in the fish. Moreover, in the experimental infection with viral hemorrhagic septicemia virus (VHSV) to the fish exposed to HO, we obtained higher mortalities in dual stressor group (virus infection with HO exposure) than those in control groups. In this study, we investigated the mechanisms of disease occurrence in the fish given the dual stressor by microarray experiment and dynamic of viral replication in the host fish. After applying stress to the fish by each single stressor or by the dual stressor, the mortalities of the groups were calculated and the live fish were dissected for sampling of kidney for the microarray experiment and heart for virus titration. As the results, fifty percent of the fish died in the dual group, while no mortality was observed in single stressor groups as well as in control. These results indicated that the dual stressor induced lethal effect in the fish, even when each single stressor had no effect. To investigate if the mortality in the dual group attributed to viral hemorrhagic septicemia (VHS), we measured the virus titre in the heart sampled from each group. The infectivities per g heart tissue were higher in dual group (105 to 108.25 TCID50/g) than those in VHSV group (103 to 106.8 TCID50/g). This suggests that VHSV easily replicates in the fish affected by the dual stressor, and a cause of death is VHS in the group. From the results of microarray experiment, the expressions of antiviral activity related genes such as interferon and apoptosis induction were relatively lower in the dual group compared with those of VHSV infection group. These results supported the high virus titre in the fish given the dual stressor. In conclusion, interferon production in the virus-infected cells and apoptosis induction by NK cells worked in a normal manner in the VHSV-infected fish without HO exposure, but these antiviral activities were suppressed in the fish affected by the dual stressor, which might lead to extensive viral replication in the host cells, resulting in the occurrence of VHS.

RA17B-6
Interactive mixture toxicity effects of a cyanobacterial stressor and insecticides may partly be grouped according to insect mode of action
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We investigated mixture toxicity of a harmful cyanobacteria (i.e., Micorcystis aeruginosa) and insecticides with different modes of action to Daphnia pulex. The widespread occurrence of such toxic cyanobacterial blooms has become an important concern for aquatic ecosystems. In agricultural areas, these toxins may act in combination with plant protection products, including insecticides. In order to study such combined effects, we exposed the waterflea Daphnia pulex to binary mixture combinations of Microcystis and 8 insecticides for a period of 21 days according to a modified central composite design. Results were statistically analyzed with the concentration addition and independent action reference models to test for additive, synergistic or antagonistic mixture toxicity. Synergistic effects were observed on reproduction for the combination endosulfan and M. aeruginosa while fenoxycarb, imidacloprid and spinosad caused synergistic effects on length in combined with M. aeruginosa. Linking the results with the mode of action, we observe no interactive effects in combinations with insecticides affecting the acetylcholine pathway by inhibition (carbaryl and chlorpyrifos). However, synergistic effects on daphnid size are observed with those insecticides that affect the acetylcholine pathway by agonistic or allosteric activity (imidacloprid and spinosad). Although endosulfan has a different molecular target compared with imidacloprid and spinosad, both of these receptors belong to the same superfamily of Cys-loop ligand-gated ion channels. This could explain the common observation of synergistic affects in all combinations with these three insecticides. Combination of tebufenpyrad and M. aeruginosa resulted in antagonistic effects on both length and reproduction. Interestingly, both can affect the oxidative phosphorylation through completely different mechanisms. Tebufenpyrad specifically inhibits electron transport in mitochondrial complex I while Microcystis is known to to affect the mitochondria. More research is needed to verify whether the antagonistic effects on reproduction are the results of combined antagonistic effects in the mitochondria. These results suggest the existence of potentially complex interaction patterns between insecticides and harmful cyanobacteria, which may require consideration in future risk assessment of insecticides in the context of climate change.

RA18 - Oil spill effects and risk assessment

RA18-1
Risk of severe oil spills - was deep water horizon an outlier?
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Following the explosion of the drill rig Deep Water Horizon (DWH) on April 20, 2010 that killed eleven workers, an estimated 670000 tons of oil were spilled in the Gulf of Mexico until the well could be capped on July 15th. This makes DWH the largest single unintentional spill in the history of drilling for oil.
Based on global data of oil spills since 1974, we estimate the expected return frequencies of such very severe oil spill events for different spill sources throught the oil chain to answer the question if the DWH spill can be considered an outlier.
This is particularly important in view of the rapid increase in deep and ultra-deep offshore activities, where both a geographical expansion as well as a trend towards drilling at ever greater depths can be seen over the last decade.
We also compare the risk of oil spills from offshore drilling with the risk of spills that is posed throughout the entire oil chain, separately for different infrastructures such as pipelines, tanker ship transport and storage. Data is extracted from our uniquely comprehensive global Energy Related Severe Accident database (ENSAD) that contains accident data from a large number of different sources. The severity is modeled with a generalized Pareto distribution, to measure specifically the risk of very severe accidents. The results give a mean return frequency based on historical data since 1974 of spills from offshore platforms and rigs exceeding the 670000 tons of the of the Deep Water Horizon oil spill of around 19 years with 5% and 95% quantiles of 7 years and 49 years respectively. Based on this result this accident cannot be considered an outlier.

RA18-2
Where has all the oil gone? Identification and toxicity of oil degradation products
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Oil is a highly complex mixture containing hundreds of thousands of compounds. Recent analyses using two-dimensional gas-chromatography - mass spectrometry (GCxGC-MS) of the acid-extractable fraction of oil sands process-affected waters (OSPW) from Alberta Canada has shown that even hydrocarbons thought to be extremely resistant to biodegradation will eventually be converted to acid products. Some of these so-called 'naphthenic acids' (NA) also have also been identified in extracts derived from crude oils and therefore likely also occur in the environment as a result of degradation of oil following accidental spillage. Previously we have reported quantitative structure-activity relationships for several structural groups of individual NA using a standard microbial toxicity assay. Now we present the toxicity of individual NA when combined as mixtures. For oil-industry produced waters, marine species may be exposed to these acids. We have now tested the effects of acute exposures to three commercial preparations of NA (CNA) on marine mussels. Many NA are not available in sufficient quantities for toxicity testing. Consequentially, we have modelled the toxicity of over 50 acids for a large number of environmental endpoints (e.g. fathead minnow lethality) and an array of human health measures such as endocrine disruption.
Structural class mixtures of individual NA plus a 35-component mixture was tested using the Microtox[TRADEMARK] assay. Mussels, *Mytilus galloprovincialis*, were exposed for 72h to three CNA and their clearance rates measured. The toxicity of 54 NA, reported to were modelled for a range of both environmental and human endpoints. The results of microbial toxicity tests of NA mixtures were consistent with a narcosis mode of action and concentration addition. This suggests that most of the compounds present in OSPW and CNA were contributing equally to their overall narcotic toxicity. The toxicity of CNA to *V. fischeri* has previously been shown to be greater than that of OSPW. Our tests now show that mussels are more sensitive to CNA than *V. fischeri*. The models predicted some NA to be several orders of magnitude more toxic to fathead minnows than other structures. In addition, some steroidal-type structures were predicted to be endocrine disruptors. When oil degrades in the environment it does not simply disappear. Instead, many hydrocarbons are converted into complex mixtures of acids that are water soluble and toxic to a range of species.

RA18-3
Use of ecosystem service valuation in quantifying ecological impacts and compensatory restoration associated with oil spills in the environment
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Since the Exxon Valdez spill, approaches to quantifying the potential impacts of an oil spill on the environment have evolved significantly. These approaches were derived out of the need to make the public whole for impacts to the environment. The approaches evolved from a strict monetary compensation framework to an ecosystem service based compensation process. That is, given that there was an impact on the environment, impacts to ecosystem services (ecological and human use services) were to be quantified and then, based upon the lost ecosystem services, the public was to be compensated by the provision of an equivalent amount of ecosystem services through the

implementation of site restoration projects. As such, the compensation (restoration) was scaled to the level of injury. This overall approach is termed the service-to-service or restoration-based compensation approach.
The author's experience, through the response and/or damage assessment phases on over 20 releases, provides insight into the methods and approaches used to quantify the impacts to the environment as well as the benefits associated with site restoration. Key ecological service quantification methodologies include the habitat equivalency analysis (HEA) and resource equivalency analysis (REA) approaches. HEA is an economic method of assessing natural resource injuries and compensatory restoration and is increasingly being used in damage assessment cases. The HEA model attempts to (1) quantify the change in service flows over time from ecological resources that have been injured, and (2) determine how much of a similar asset must be preserved, created or enhanced to provide an equivalent flow of services to those that were injured. Although the author will focus on the application of the HEA approach to evaluate ecological service losses, they will also touch on human use impact analyses that are typically conducted by a variety of standard economic approaches. The author will discuss both the debit and credit calculation phases as they relate to the evaluation of impacts associated with an oil release and the scaling of an appropriate level of restoration (compensation). This presentation will provide an overview and case application as to how these methodologies have been used to quantify impacts and scale restoration as the result of oil spills. Case examples will be provided.

RA18-4
Effects of chemically and mechanically dispersed oil on fitness-related and molecular endpoints in the North Atlantic copepod Calanus finmarchicus
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In recent years there has been an increasing emphasize on the significance of invertebrates for assessing environmental impact of oil spills. In the event of accidental oil spills in sub-Arctic and Arctic marine environments planktonic organisms like copepods are realistic targets for oil toxicity based on their significant role in the food web, their abundance and their large lipid content. For many years the SINTEF/NTNU culture of Calanus finmarchicus has functioned as relevant model for standard ecotoxicity testing of North Atlantic crude oils, and a large database of ecotoxicity data exists for this species. Parameterized experimental data on the effects of oil (single oil components, water soluble fraction of oil, and dispersed oil) on copepod survival and reproduction are used as input for development of numerical models for environmental risk and damage assessment. The accessibility of a continuous copepod culture provides homogeneous specimen in terms of developmental stage and lipid content. This, along with sophisticated experimental systems, is a major foundation for investigating effects of stressors on molecular systems. A 15K oligonucleotide microarray has been developed based on 260,000 ESTs sequenced using FLX454 technologies. Several methods, like 1H-nuclear magnetic resonance and mass spectrometry, have also been developed and applied in order to investigate metabolic profiles and alterations. Together these complementary methods give valuable supporting information to well known fitness-related endpoints, as they contribute with modes of toxic action of stressors, and output data may also be used to determine effect limits. The presentation will include results from an experiment aimed at comparing the effects of chemically and mechanically dispersed oil, their modes of toxic action, and proposed effect limits of toxicity based on fitness-related endpoints as well as molecular profiling. These data will provide input to environmental models for risk and damage assessment following acute oil spills.

RA18-5
Temperate and polar marine species sensitivity to oil components in relation to accumulation kinetics
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Risk assessments for polar marine ecosystems are mostly based on toxicity data obtained for temperate species. Yet, it is unclear whether toxicity data of temperate organisms can be used to derive reference values for protection of polar species, as differences in physiological characteristics, like metabolism and lipid composition, may yield differences in sensitivity to toxicants. The first aim of our study was therefore to compare polar and temperate marine species on their sensitivity to oil. To that end, species sensitivity distributions (SSDs) were constructed for crude oil, 2-methyl-naphthalene, and naphthalene based on acute toxicity data from scientific literature and databases. To allow for an estimation of the overall risk of oil contamination in the field, toxicity thresholds of oil components are needed. Therefore, our second aim was to model oil toxicity based on accumulation and transformation of oil fractions in marine organisms and to validate the outcome by comparison with lab and field measurements. LC_{50} values (lethal concentration for 50 % of the organisms) were calculated by using a critical body residue for compounds acting by narcosis and a weighted average of log octanol-water partition ratios (K_{ow}) of the individual components constituting oil.
The HC_{50} value (hazardous concentration for 50% of the organisms) and estimated LC_{50} value for naphthalene, 5.0[GREEKX]10^3 µg/l and 5.7[GREEKX]10^3 µg/l respectively, showed little difference. Therefore, the average toxicity of naphthalene to temperate marine species can be predicted based on accumulation kinetics. A K_{ow} of 10^4 and molecular mass of 200 yielded an LC_{50} of 2[GREEKX]10^3 µg/l for oil in general. A more refined calculation taking into account biotransformation and specific modes of action underpinned this value.
The sensitivity of polar and temperate marine species to oil and oil components differed on average less than a factor of 3. In addition, most of the differences were not statistically significant and there was no taxonomic group that was consistently more sensitive than the other groups. Apparently, physiological mechanisms suggested to cause differences between polar and temperate species have little overall effect on sensitivity to oil. As a consequence, toxicity data obtained for temperate organisms may serve to obtain a first indication of the risks in polar regions. Yet, exceptions may result from biotransformation and specific modes of action.

RA18-6
Integrating marine physics, biological and eco-toxicological models into a unified simulation system for oil spill risk and impact assessment
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A 3-year project called SYMBIOSES has been initiated to develop a holistic, integrated modeling framework for ecosystem-based risk and impact assessments. The strategy is to couple existing numerical models, each of which has been previously tested, validated, and proven useful. This approach avoids the cost of basic code development and testing, but introduces different challenges in that the various components are based on quite different numerical solution methods. The system consists of physics, biological, oil/chemical fates and eco-toxicological components. The physics models are Eulerian, as are some of the biological models, whereas the pollutant fates and some of the biological components are Lagrangian. The related process equations of the component models are solved in general on different time-steps, and at different spatial resolutions. The design of the system requires the possibility of two-way communication between model components (e.g. zooplankton feeding on phytoplankton, zooplankton consuming oil droplets of appropriate size, chemical concentrations affecting growth of phytoplankton, mortality, growth and reproduction of zooplankton, and growth and mortality of ichthyoplankton). It is also desirable that alternate components can be inserted into the system, to facilitate geographic transportability as well as uncertainty analyses. We therefore seek a relatively flexible and transparent set of methods to achieve integration of the separate models into the system. We assume that the basic physics models are always Eulerian: regardless of numerical solution, the computations are carried out on a regular or irregular grid that is spatially fixed for the duration of a given simulation. The biological and oil/chemical transport and fates models may be either grid-based or particle-based (pseudo-Lagrangian), and will in general produce data on spatial scales different from that of the physical basis models. This paper will describe the proposed design plan to meet these challenges.

RA19 - Plants and chemicals in the environment: risk assessment, pest management and phytoremediation

RA19-1
Risk assessment of herbicides for the common buttercup Ranunculus acris in field margins - an experimental field study
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Field margins comprise the majority of semi-natural habitats in the intensively farmed agricultural landscape and thus they can benefit the conservation of biodiversity in agroecosystems. However, field margins can be affected by pesticide by direct overspray and spray drift from field applications. The risk assessments of herbicides are often performed with single and annual plants species in early development stages in greenhouse experiments. But the vegetation of field margins usually consists of annual and perennial plant species in different development stages. Also an insufficient knowledge about the sublethal and long term effects of herbicides on plants is available.
The present perennial field study (start 2010), was undertaken to investigate the effects of repeated herbicide applications in successive growing seasons on *Ranunculus acris* in field margins. The test design followed a randomized block design (7 treatments, 1 control, 8 replicates). The applications of the treatments and their application sequences mimic the field management of winter wheat fields with their recommended agrochemical products and application rates. The applied fertiliser and pesticide concentrations

are consistent with their inputs (drift+overspray) in the first meter of a field margin directly adjacent to a field under Good Agricultural Practices.
To detect the effects of the applications vegetation assessments and a photo-documentation of the flower intensity of *R. acris* was performed in May 2010 and 2011. Additionally the experiment was accompanied by monitoring of *R. acris* in field margins in the study area in May 2011.
R. acris revealed sublethal effects after the herbicide applications. Flower intensity was significantly reduced in the herbicide treated plots, whereas plant presence was not affected. So far these sublethal effects are not accounted for in risk assessment procedures. However in the long run these effects will cause the decline of specific plants and set in community shifts in agricultural field margins. This was confirmed by the monitoring where *R. acris* could hardly be observed in field margins adjacent to cereals, whereas in field margins located next to pastures or orchards (no herbicide use) the species was recorded more frequently. Besides the implications for the plants the described sublethal effects can also cause secondary effects for flower visiting arthropods and thereby negatively affect the biodiversity of the agricultural landscape.

RA19-2
Enhancing risk assessment by using a toxicokinetic and toxicodynamic (TK/TD) growth model of Myriophyllum spicatum
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Toxicological studies used for risk assessment can only cover a limited range of exposure scenarios due to their work intensity. Ecological models considering the toxicokinetic and toxicodynamic of chemicals are capable to close the lack of exposure scenarios in toxicological studies and, thus, enhance risk assessments by predicting the effects of variable exposure scenarios.
In this work a toxicokinetic and toxicodynamic growth model of Myriophyllum spicatum is presented giving the ability to predict the effects of chemical substances on the growth of M. spicatum. Therefore, a growth model considering the most important factors influencing the growth was developed. A toxicokinetic part calculating the uptake and elimination of chemicals depending on their physicochemical properties and the physiology of M. spicatum was included in the growth model. Moreover, a toxicodynamic part using the internal concentration in M. spicatum and experimentally established dose-response relationships to modulate the growth rate of M. spicatum was added to the model. The model is able to predict reversible growth inhibition under different environmental and exposure conditions based on standard test results.
The model was verified with experimental data on growth inhibition of M. spicatum after fourteen days due to different concentrations of 3,5-dichlorophenol (DCP). The model was able to predict the effect of 3,5-DCP exposure on M. spicatum very well but cannot fully explain the total inter experiment variability of growth, particularly under untreated conditions. The model can be used to predict growth inhibition for 3,5-DCP. Further validation and verification of the model is needed to ensure that the model works properly and to show that the model can be used for a wide range of substances with different physic-chemical properties.

RA19-3
Herbicide impacts on macrophytes: can we predict community-wide effects from single-species toxicity tests?
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RA19-4
Linking aquatic plant toxicity data for pesticides to risk assessment endpoints and environmental protection goals
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This presentation discusses protection goals for aquatic plants, assessment endpoints that address those protection goals, and the relationship of standard toxicity data to the assessment endpoints and protection goals. Protection goals for aquatic plants generally focus on the plant community as a whole, rather than particular species or individuals as is the case for aquatic animals. Consistent with these protection goals, it is not necessary to completely protect every sensitive plant species; protecting some fraction of plant species (represented by a certain percentile of the Species Sensitivity Distribution, SSD) is sufficient to protect overall community function and structure. Assessment endpoints used to characterize effects of chemicals on aquatic plants should represent inpacts of similar severity to assessment endpoints used for animals, in relation to their respective protection goals. Toxic endpoints for aquatic plants are based on non-lethal responses, unlike acute endpoints for animals which are based on mortality. Furthermore, aquatic plant communities usually recover more quickly than animal populations (especially fish) from effects of stressors. These considerations suggest that assessment endpoints for aquatic plants should be based on a higher SSD percentile than the 5% typically used for animals. When data are unavailable for a sufficient number of species for SSD analysis, a small number of surrogate test species (Lemna gibba, Myriophyllum spicatum, and certain algae) can indicate the toxicity of herbicides and fungicides to the most sensitive aquatic plants.

RA19-5
Uptake and intra-cellular accumulation of hydrophobic chemicals in charophytes and implications for ecosystem exposure control and remediation
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Uptake to primary producers (constituting an important pool of organic carbon in lakes) is a key step for addressing hydrophobic chemicals to upper trophic levels. It has been hypothesized that permeation and diffusion through biota surface structures such as epitelia, cell walls or membranes may be inhibited for highly hydrophobic substances by steric hindrance of membrane passage. Chara rudis is a macroscopic, perennial, benthic taxon having a protective layer of cortex cells. We used 14C12 radiolabelled Hexachlorobenzene (HCB) to i) investigate whether or not HCB can reach the internode cell, ii) to assess the distribution of HCB in different plant parts, and iii) to discuss the implications of the accumulation on benthic macroalgae for fresh water ecosystems. We found that i) about 65% of the total amount of HCB added to the microcosm was associated to the algae tissues, ii) the HCB in the cortex cells represented about 90 to 95% of the total found in the plant, and iii) HCB was detected at measurable levels in 57% of the sampled internode cell cytoplasm, demonstrating the occurrence of intracellular transport and storage of chemicals. In some water bodies charophytes grow in very dense meadows up to 2m tall and can cover a large fraction of the water body bottom. The high efficiency of taking up hydrophobic chemicals directly from the water phase suggests that they can also represent a key control for the mass balance of POPs in the water ecosystem wherever they are abundant.

RA19-6
'Halophyte filters': the potential of using halophyte species for phytoremediation purposes in saline aquaculture
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There is a growing consumer demand for seafood as protein source, and land-based (marine) aquaculture is seen as a sustainable way to meet this growing demand. A major problem with aquaculture is the nutrient waste, since most of the nutrients added through feed are released into the environment, predominantly in dissolved form. Filtration and sedimentation techniques to reduce nutrient concentrations are not adequate for the large volumes of waste water produced in aquaculture. The use of constructed wetlands has been shown to be successful in freshwater aquaculture practices. Freshwater constructed wetlands are worldwide used to treat various types of wastes. However, there is only limited experience in saline systems. The main aim of this study is to analyse the potential of constructed saline wetlands in land-based marine aquaculture.
The main advantage of using wetlands is that these are relative simple systems that need little control after construction. The location of the wetland can be located close to the source, limiting transport of waste water through pipelines. Further, wetlands can simultaneously reduce several contaminants (BOD, suspended solids, nutrients, pesticides, pathogens). The primary function of a constructed wetland is the purification of water, but there are also several ancillary benefits that can be incorporated in wetland treatment designs. For example a high vegetation biodiversity, offering a habitat for fauna, and giving aesthetic, recreational, commercial, and educational human uses. Different approaches exist to utilize plants (halophytes, macro-algae, micro-algae) in the treatment of marine aquaculture effluent; these are described in a conceptual framework. In essence, all the approaches attempt to maximize the ecosystem service of water purification. The approaches differ in the balance between economic benefits and nature benefits. The potential use of this framework is demonstrated with a Dutch case study.

RA20 - Risk assessment of chemical mixtures: where do we stand? what are the next steps?

RA20-1
Predictive regulatory risk assessment of chemical mixtures in the aquatic environment: a conceptual framework
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Risks of chemicals in the aquatic environment are still often assessed substance-by-substance, neglecting mixture effects. This may result in risk underestimations, as the typical exposure is towards multi-component chemical "cocktails". We used the two well established mixture toxicity concepts of concentration addition (CA) and independent action (IA) for developing a tiered scheme for environmental hazard and risk assessments of mixtures, focusing on general industrial chemicals regulated in the EU under REACH and assuming that the so-called "base set"of toxicity data is available, i.e. EC50 values for algae, crustaceans, and fish.
As mixture toxicities higher than predicted by CA are rare findings, we suggest applying CA as a precautious first tier - irrespective of the modes of action of the mixture

components. In particular, we show that summing up PEC/PNEC ratios might serve as a justifiable CA-approximation, in order to extrapolate from the "base set"data to the aquatic ecosystem in a regulatory first tier assessment. This approach makes optimum use of already existing single substance assessments. More in-depth mixture investigations may be requested only if the first tier estimates give an indication of a potential environmental risk. Finally we suggest to call for mode-of-action driven analyses only if error estimations indicate the possibility for substantial differences between CA- and IA-based assessments.

RA20-2

Bearing down the borders? - Considerations on an environmental risk assessment of substance combinations across different regulations

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Across Europe, the prospective environmental risk assessment (ERA) of chemical substances is conducted under separate regulatory frameworks, i.e. for plant protection products, biocides, industrial chemicals as well as human and veterinary pharmaceuticals.
The aim of this prospective assessment is to avoid adverse effects of these chemicals a priori to an exposure of the environment. Under all regulations, the current assessment methods focus on single substances only. As it is well accepted that multiple substances typically reach environmental compartments together and act jointly on organisms, strategies and methods for an assessment and regulation of chemical mixtures are currently under development for all these regulatory frameworks.
The presentation focuses on the activities at the "Chemical and Biological Safety"Division of the German Federal Environment Agency (Umweltbundesamt, UBA) with a focus on the development of common methods and strategies for the consideration of substance combinations under the different legislations. Furthermore the limitations and needs for an assessment of mixtures that reach the environment from multiple sources, i.e. substances that traditionally fall under different legislations, are pointed out. Existing approaches for overarching concepts beyond substance-oriented regulations are discussed from an regulatory perception. Common agreements on definitions, assessment methods and strategies across the substance-oriented regulations are important. The same applies for an exchange of knowledge and data between regulations, which would enable an assessment of substances from a variety of sources. Overarching concepts might be helpful for certain situations and substances, but it needs to be clarified for which cases and who might conduct such an assessment.

RA20-3

The threshold of (eco)toxicological concern: a suitable tool for mixture risk assessment and ranking?

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The threshold of toxicological concern is defined as a safe level: a concentration at or below which there is no appreciable risk for humans (TTC) or the environment (ecoTTC). Recently, the TTC concept has also been put forward as a tool for the risk assessment and ranking of chemical mixtures, for example in the recent opinion on mixture toxicity assessment by the scientific committees of the European Union. In particular it has been argued that compounds that are present at or below their individual (eco)TTC do not contribute to the (eco)toxicity of a mixture. That is, a mixture would pose no risk for human health or the environment, as long as all components are present only in concentrations at or below their individual (eco)TTC.
The TTC approach has a range of appealing features. It would be extremely helpful for simplifying the (eco)toxicological assessment of complex mixtures by allowing to ignore compounds below their individual (eco)TTC. It would also simplify the problem of mixture toxicity assessment to a single substance assessment, as we can safeguard against any mixture effect, as long as we can ensure that the concentrations of all compounds never exceed their individual (eco)TTC. Furthermore, the (eco)TTC seems to provide a good basis for the exposure-based waiving of risk assessment in the context of e.g. REACH. A first ecoTTC-like approach is already implemented in the form of the so-called action limit in the European guideline for the environmental risk assessment of pharmaceuticals.
I will briefly review the conceptual basis of the (eco)TTC, the suggested applications in the context of mixture toxicity assessment and will then discuss the implications of its application in view of the classical mixture toxicity concepts (Concentration Addition and Independent Action), which are the cornerstones of our current understanding of mixture (eco)toxicology. The main conclusions are that (i) the (eco)TTC concept requires constant update of the underlying (eco)toxicological data, as the chemicals in use change over time, (ii) the (eco)TTC concept needs to be adjusted for mixtures that contain at least partly compounds with a similar mode of action, which might make it primarily useful for risk management, and (iii) that in particular the ecoTTC requires further development and refinement if it is to be used in the context of ecological protection goals.

RA20-4

Long-term trends in potential toxicity of unknown organic micro-pollutants in rivers

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During these years, the effects of toxic substances on the ecosystem in Dutch inland waters were measured with a complementary method, i.e., by means of so-called bioassays. This approach provides information on the effects of unknown chemicals in water which are overlooked by traditional analytical techniques. The latter cover only a small portion of the large number of chemicals that are present in surface water. Moreover, classical chemical techniques do not give insight into the auxiliary effect that several toxic substances may have.
The results from the bioassays confirm that damage to the aquatic ecosystem during the last decade due to the presence of toxic substances has decreased. Toxic pressure in the river Rhine in the year 2000 was already very low but has decreased further. Toxic pressure in the water of the rivers Meuse and Scheldt was significantly higher than that in the river Rhine, but has decreased considerably since the year 2000. The results also indicate that the toxic pressure is higher upstream and decreases downstream.
The reaction of five organisms to toxic chemicals in a water sample was measured with bioassays. Applying the species sensitivity distribution method to this small set of data results in a snapshot of the toxic stress. This approach is however flawed by large uncertainty margins which make a series of snapshots unsuitable for discerning a trend in water quality. A trend became apparent when all bioassay results collected over the whole period were combined by means of an advanced statistical technique. As a result, information on toxic trends becomes more accurate because the multitude of data has reduced the spread in toxic stress in river water sampled at a given river bank location. Responses to the bioassays provided insight into the nature of the toxic compounds. The cocktail of toxic substances in the river Rhine was found to consist of non-polar chemicals, i.e., substances without a specific mode of action which affect all aquatic organisms. In the other rivers, pesticides are probably responsible for the observed effects. In the summer of 2002, the river Meuse must have been polluted by both known (albeit banned for more than ten years at that time) and unknown herbicides, as revealed by a comparison of chemical measurement and bioassay results.

RA20-5

Toxicity of metal mixtures to Daphnia magna: Implications for a multi-metal, multi-site biotic ligand model

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In real-world aquatic systems, organisms are usually exposed to metal mixtures instead of individual metals. To predict the toxicity of metal mixtures, we have been developing a mechanistic model based on tissue residues of metals and on the concept that the toxicity of a mixture of metals can be either dose-additive or response-additive, depending on the mechanisms of action. To calculate tissue residues and thereby predict toxicity across wide ranges of water quality, we have been developing a multi-metal, multi-site biotic ligand model (MMMS BLM) that concurrently accounts for metal-metal competition for binding on dissolved ligands in the water and at sites of toxicity on organisms. We have exposed Daphnia magna to mixtures of Cu and Zn, Cd and Cu, or Cd and Zn in moderately hard reconstituted water containing dissolved organic matter (added as Suwannee River fulvic acid) at 3 mg DOC/L, and compared observed mortality to the null assumption of additive mortality predicted from results of concurrent Cd-only, Cu-only, and/or Zn-only toxicity tests. This research has revealed several apparent metal-metal interactions that otherwise might lead to conclusions that metals interact in non-additive ways, yet simple geochemical speciation in the BLM can explain these interactions and reconcile the apparent non-additive toxicity. For example, the toxicity of Cu-Zn mixtures always appeared to be more-than-additive or additive when based on dissolved metal concentrations, whether Cu was varied while Zn was held constant, or vice versa; whereas in the same tests, the toxicity of the Cu-Zn mixtures always appeared to be less-than-additive or additive when based on free-metal-ion concentrations. In contrast to the results for Cu-Zn mixtures, the toxicity of Cd-Cu and Cd-Zn mixtures appeared to be less-than-additive or additive when based on dissolved metal concentrations. These results demonstrate that different metal mixtures can appear to interact differently based on dissolved-metal or free-ion concentrations, but a MMMS BLM could help reconcile those apparent inconsistencies and could be an effective tool to help water quality agencies implement appropriate methods to regulate metal mixtures.

RA20-6

Low dose mixture effects - detectable using toxicogenomic approaches ?

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The advent of toxicogenomic techniques have raised large expectations that some of the central questions of mixture toxicology such as for mechanisms of low dose interactions can be provided with novel perspectives if not definite answers. After the first decade of experimental studies this review summarizes mixtures toxicity studies that

address diagnostic, mechanistic or extrapolation questions. Since 2002 almost 40 studies were published with their major focus on mixture toxicity assessment by means of toxicogenomic techniques, mainly through microarray or qPCR techniques, though metabolomic and proteomic analysis of joint exposures have also been undertaken. It is now standard to explicitly state criteria for selected concentrations and provide insight into employed data transformation, and statistical treatment with respect to minimising sources of undue variation. Bioinformatic analysis of toxicogenomic data, by contrast, is still a field with diverse and rapidly evolving tools. The combined effect assessments achieved are discussed in the light of established toxicological dose-response and mixture toxicity models. Often transcriptomic responses are discussed based on the presence or absence of signals. As there are yet no consented ways of how to interpret these effects, there are ambiguous interpretations. Furthermore, mixture studies in their majority designed their experiments and compared their recorded outcomes against individual treatments i.e. focus was to retrieve signals of individual components under mixture exposure. This stands in stark contrast to our existing understanding of biological activity at the levels of chemical target interactions and apparent apical combined effects. Here models are employed to calculate expected combined effects based on information of the mixture components' individual dose-response relationships. By joining these mixture effect models with toxicokinetic and -dynamic thinking we suggest a theoretical framework that may help to overcome the current limitation of providing mainly anecdotal evidence on mixture effects and progress into more hypothesis driven mixture studies. As ways forward we suggest to study and establish quantitative relationships between dose dependency and time dependency of responses.

RA21 - Standard vs non-standard methods for hazard and risk assessment

RA21-1

Is there a need to better standardise test organisms in ecotoxicology? A case study based on sexual development in inbred and outbred zebrafish (Danio rerio)

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The use of outbred laboratory animal strains representing wild populations is often advocated but rarely demonstrated in ecotoxicology. Due to practical constraints limiting effective population sizes, laboratory animal strains are generally more inbred and less genetically diverse than their wild counterparts. Furthermore, breeding history may vary considerably between strains, driving differences in genetic variation and ultimately phenotypes used for assessing effects of chemical exposure. Developmental phenotypes are particularly susceptible to variation due to phenotypic plasticity caused by genotype[GREEKX]environment interactions. Sexual development in the zebrafish is a potential case in point. Sex determination in this species has been shown to be highly plastic and therefore influenced greatly by environmental factors (including chemical exposure), as well as genetic factors.

We compared a range of phenotypic endpoints in zebrafish from four different "breeding treatments"comprising a WIK zebrafish strain and a WIK/Wild strain with three levels of inbreeding (FIT=n, n+0.25, n+0.375) in the new OECD234: Fish Sexual Development Test (FSDT), where one of the core endpoints is sex ratio. There were no differences between treatments in terms of egg viability, hatch success or fry survival. However, compared with WIKs, WIK/Wild hybrids were significantly larger in size with more advanced gonadal (germ cell) development at the end of the test. Increasing the levels of inbreeding in the related WIK/Wild lines did not affect body size, but led to a male bias (72%) in the most inbred line (FIT=n+0.375). Conversely, in the reference WIK strain there was a significant female-bias in the population (80% females). Overall, our results support the use of outbred zebrafish strains in the FSDT. Despite increased variance in some endpoints, WIK/Wild outbreds (FIT=n) met all acceptance criteria for controls, whereas WIKs failed to comply with tolerance limits for sex ratio (30-70% females). Sexual development was also more advanced in WIK/Wild outbreds (c.f. WIKs), providing greater scope for detecting developmental toxicity following chemical exposure.

Whilst considerable attention is paid to the standardisation of environmental conditions in test guidelines, pedigree and/or genetic information confirming the use of outbred strains in ecotoxicology is generally lacking. This additional information should aid further standardisation of regulatory studies.

RA21-2

Improved protocols for sediment toxicity testing: a review

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At present, tests to assess the toxicity of sediment-bound chemicals to sediment-dwelling organisms are relatively well established for a few test species. However, there is a lack of cost-effective and widely accepted methods to assess potential effects on microorganisms, macrophytes and animals across taxonomic groups, as well as methods to translate results of such tests between freshwater and marine ecosystems and to the population and community levels. Such methods, however, are crucial within the current context of criteria setting and prospective risk assessment (PRA). Here, we critically review the state of the art on prospective sediment toxicity testing with individual organic compounds in order to identify knowledge gaps and to provide guidance for optimum sediment toxicity test designs for microorganisms, macrophytes and benthic invertebrates. Focus is on freshwater, estuarine and marine systems in the temperate zone, however also with relevance for other climate zones. We synthesise an overview of recommendations from the literature on sediment preparation and spiking, microorganism, macrophyte and invertebrate tests, microcosm and mesocosm tests in the regulatory context and framework of PRA.

Standard test protocols are only available for benthic invertebrates, whereas a protocol for the freshwater macrophyte Myriophyllum sp. is currently under development. Tests for macrophytes, invertebrates and microorganisms to a lesser extent are described in the literature but prospective micro- and mesocosm tests are rare and highly diverse. Compared to freshwater sediment tests, marine and estuarine tests have received much less attention. In order to perform a proper sediment toxicity test, it is recommended to use spiked artificial sediment and artificial water, assess exposure by passive sampling and use selected test species. Standard species together with optimized standard test protocols form the basis of an improved first tier of sediment PRA.

RA21-3

Use of public literature and dossier data in WFD EQS derivation compared to risk limit derivation in other regulatory frameworks

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In the Netherlands, RIVM has a broad experience on both the derivation of Environmental Quality Standards (EQSs) under the Water Framework Directive (WFD) and the evaluation of dossier data within various regulatory frameworks. An overview will be given of the use of public literature in EQS derivation, which will then be compared to the use of public literature in the derivation of risk limits, e.g. PNECs, in REACH and the framework of plant protection products.

For EQS derivation according to the draft guideline of the WFD, all relevant available information should be considered. This means that dossier data submitted under the relevant frameworks should be used, but also data from open literature should be included, provided that the scientific reliability is sufficient and endpoints are relevant. For reliability, the scores of Klimisch [2] are used, with a division into four categories: 1 = reliable; 2 = reliable with restrictions; 3 = unreliable; and 4=unassignable. Only studies with a validity score of 1 or 2 can be used for EQS derivation. However, not all valid studies are also relevant for EQS derivation. Only endpoints which are relevant to the population should be taken into account. Thus, endpoints like histopathology, blood parameters, general activity, swimming speed, organ weight and results from in vitro tests cannot be used for EQS derivation, even if this would result in more critical values.

The use of public literature differs among the various frameworks, partly because of the specific guidelines but also because public literature cannot always be assessed for its validity. The use of public literature in regulatory framework risk assessments could seriously improve if all relevant methodological details would be described and results are reported in a clear way. Then, even if a study is not performed according to OECD guidelines or GLP, it could still be used for EQS derivation and other regulatory work. The datasets used may differ among the frameworks, not only because of different ways of literature searching, but also because of diverging choices made in assessing reliability and relevance This means that EQSs and PNECs may be focussed on the same protection goal, but they can numerically still differ among frameworks. The challenge is to harmonise the data sources used and ensure enough transparency so that data can be used across all frameworks, irrespective if industrial or governmental parties derived the risk limit.

RA21-4

Standard and non-standard ecotoxicity tests in regulatory risk assessments of chemicals

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Guidance documents recommend the use of standard ecotoxicity tests in regulatory risk assessments [1-6]. These recommendations have decreased the use of non-standard test data for several groups of chemicals. On the positive side, this has increased the reliability of the data since the strict reporting requirement for standard tests enhance reliability. On the negative side, it could have implications for the relevance of the risk assessment. Standard tests may not always be sensitive enough to measure the specific effects expected for instance from endocrine disrupting chemicals, nanoparticles and pharmaceuticals. Bisphenol A is an illustrative example since three standard tests are preferred by several risk assessors over 200 non-standard studies with lower effect values [7].

Previous studies indicate that ecotoxicity studies published in the open scientific literature are surprisingly often insufficiently reported [8]. This may be a major reason why they are often seen as less reliable in a risk assessment context. Choice of reliability evaluation method could also affect the outcome of the evaluation [8]. Several guidance

documents recommend that the method described by Klimisch et al. [9] should be used for evaluating the reliability of ecotoxicity and toxicity data but the Klimisch criteria give a strong preference for standard tests.
We present a novel and more comprehensive method for evaluating and reporting non-standard ecotoxicity data [10]. Its aim is to enable an increased use of non-standard data in risk assessments. As part of this work we clarify the definitions of "reliability"and "relevance"in order to promote the consistent use and application of these concepts in risk assessment procedures. Lastly we present examples from environmental risk assessments of pharmaceuticals showing how non-standard data can complement standard data to arrive at robust and transparent risk assessments.

RA21-5
Toxicity and detoxification of chemicals in detergents, softeners and shampoos
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Previously environmental concern was mainly focused on the intentional release of chemicals from use of pesticides and discharges from industries. Presently concern has also been raised on non-intensional release of chemicals from articles and products like paints, textiles, tires, plastics, pharmaceuticals, and personal care and cleaning products. For all chemicals their hazard and risk is based on toxicity (including genotoxicity and sensitation), degradation and bioconcentration, either from real testing or chemometric modelling. However, for products and articles, which may contain many chemicals at confidential concentrations, assessments of biodegradation, bioconcentration and combined toxicity based on ingredient toxicity are not possible to make. Therefore, an approach similar to that used for industrial wastewaters using toxicity testing and, when necessary, TIE (Toxicity Edentification Evaluation) might be used. Since many chemicals will reach the environment via sewage treatment works, their biodegradation and detoxification are important for their environmental ecotoxicity. Reseach on detergents, softeners and shampoos has shown that surfactants are key chemicals for the toxicity of these products, and that there is a wide range in product toxicity, as well as in their detoxification. Recent studies, using the standard ISO test with Daphnia (ISO 6341) and innoculation by activated sludge, have shown that toxicity (24-h EC50) have ranged from 4 to 1615 mg L-1 for 26 detergents, from 25 to 225 mg L-1 for 5 softeners, and from 0.54 - 163 mg L-1 for 9 shampoos. This variation suggest that there is a considerable potential for toxicity reduction among these products either through replacement of entire products or by chemical substitution. The former needs more transparency of environmental labelling and a more sophisticated labelling into more than one category. The latter implies a better communication and co-operation between academia, industry and regulators. Recent research on detoxification has shown a wide range also in detoxification and differences between products in abiotic (without activated sludge) and biotic (with activated sludge) degradation. Even if the reasons for all variation is not known it is obvious that this aspect should be considered together with toxicity in the hazard and risk assessment.

RA21-6
Aquatic toxicity of halogen-free flame retardants
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Several halogenated flame retardants have been banned due to their persistence, bioaccumulation potential, toxicity (PBT) and probable environmental risk. Hence, alternative flame retardants are required and a range of new flame retardants have been proposed. The PBT properties of most alternative flame retardants are, however, poorly characterized. Therefore, the aim of the present study was to make an inventory of the available data on aquatic toxicity of a selection of halogen-free flame retardants (HFFRs) that are already commercially available. The data were classified according to the REACH system, meaning that we assigned the categories "high", "moderate"and "low"(< 1 mg/L, 1-10 mg/L & > 10 mg/L respectively). Since data gaps exist, the acute aquatic toxicity to *Daphnia magna* was determined for the selected compounds.
To determine the EC50 values, the compounds were subjected to 48 h immobility tests with Daphnia magna, based on OECD guideline 202. For each compound, first the concentration that equals the maximal water solubility (max. Sw) was tested. Second, if an effect was observed at max. Sw, a dilution range was prepared (4 concentrations per compound) and tested to determine the EC_{50}. The alternative flame retardants studied included six organic phosphates (Aluminium Diethyl Phosphinate (ALPI), Bisphenol A bis(diphenyl phosphate) (BDP), Dihydro Oxa Phosphaphenanthrene (DOPO), Melamine Polyphosphate (MPP), Resorcinol bis(diphenyl phosphate) (RDP), Triphenyl Phosphate (TPP) and six inorganic compounds (Aluminium Trihydroxide (ATH), Ammonium Polyphosphate (APP), Antimony Trioxide (ATO), Magnesium Hydroxide ($Mg(OH)_2$), Zinc Hydroxy Stannate (ZHS) and Zinc Stannate (ZS)). Tetra bromobisphenol A (TBBPA) was tested as well, as a reference compound for halogenated flame retardants. TPP and TBBPA had a high toxicity to *D. magna*. In contrast, the literature review revealed that ATO, APP and ZHS did not show high aquatic toxicity. Also, these compounds and $Mg(OH)_2$ and ZS showed low acute toxicity to *Daphnia magna*. Therefore, these compounds were considered here to be the most promising HFFRs. However, the review showed as well that for these compounds still large data gaps exist. To assess whether the presently studied HFFRs are actual viable alternatives, these gaps should be filled and each compound should be examined individually by comparing its toxicity values with those of the relevant halogenated flame retardant.

RA22 - The use of rodenticides, a nagging issue on effectiveness and risks

RA22-1
Anticoagulant rodenticide uptake in resistant rat populations
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Anticoagulant rodenticide (AR) resistance in rat populations has been a problem for fifty years. However, its impact on non-target species, particularly predatory and scavenging animals has received little attention. Field trials were conducted by RRAC on farms in Germany and by the University of Reading on farms in England, where resistance to anticoagulant rodenticides had been confirmed. Resistance is conferred by different mutations of the VKORC1 gene in each of these regions: tyrosine139cysteine in Germany and leucine120glutamine in England. A modelling approach was used to study the transference of the ARs into the environment during AR treatments for Norway rat control. Baiting with brodifacoum resulted in lower levels of AR entering the food chain via the rats and lower numbers of live rats carrying residues of AR during and after the trials due to its effectiveness against resistant rats. Bromadiolone and difenacoum resulted in markedly higher levels of AR uptake into the rat population and more live rats carrying residues during the trials and for long periods after the baiting period. Neither of these compounds provided full control on any of the trial farms. Secondary non-target predators were predicted to take up more AR when residues in rats were higher and the more rats remained alive. In resistant areas where ineffective compounds are used there is the potential for higher levels of AR exposure to non-target animals, particularly predators of rats and scavengers of rat carcasses. Thus, resistance influences the total amount of AR available to non-targets and should be considered when dealing with rat infestations, as resistance-breakers may present a lower risk to wildlife.

RA22-2
What do anticoagulant rodenticide residues in predatory birds and mammals tell us about non-target exposure and risk?
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Anticoagulant rodenticides (ARs) are non-specific in their toxicity and so liver residues have been measured in non-target species to gain information on scale of exposure and to assess the likelihood of effects. The second-generation anticoagulant rodenticides (SGARs) have been a focus for monitoring because their widespread use, high acute toxicity and persistence enhance potential for secondary exposure and poisoning. We review what monitoring has told us about the key factors that mediate exposure of non-target species and the likelihood of adverse effects.
Exposure of predatory birds and mammals to SGARs is widespread but species vary in their accumulation of liver residues. *Diet* is assumed [but rarely shown] to be a major factor yet significant differences in residue accumulation occur between species with similar diets. However, a recent study strongly suggests that diet can indeed be a key factor. When prey guild is restricted, foxes (*Vulpes vulpes*) feed relatively extensively on commensal rodents and other species likely to take AR bait. As a result, they accumulate greater SGAR residues than animals from areas where prey choice is wider and includes species unlikely to encounter bait. *Usage* is also likely to influence exposure. At large spatial scales, the overall pattern of wildlife exposure reflects SGAR usage but the relationship between use and exposure appears more complex at a local scale. The way SGARs are used, rather than the total amount used, is likely to be of prime importance. *Resistance* to ARs in commensal species may also affect exposure in predators. Resistant rats survive (and are available to predators) for longer than non-resistant individuals and may also accumulate higher AR body burdens. The importance of resistance in mediating exposure and risk remains a key question. It can be addressed through analysis of wildlife residues but first requires that resistance areas are mapped.
The relationship between magnitude of liver residue and likelihood of mortality in wildlife is poorly defined. A "potentially lethal range"has been proposed for barn owls (*Tyto alba*) but is poorly defined, not diagnostic and may vary between ARs and species. New probabilistic analyses to assess the likelihood of mortality associated with any given AR residue offers an exciting new approach that may allow, for the first time, estimation of likely toxicity at a population level and identify inherently sensitive species.

RA22-3

Reflections on the risk of first generation Anticoagulant Rodenticides to Raptors

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In 2008, the United States Environmental Protection Agency placed new regulatory restrictions on the use of second generation anticoagulant rodenticides. These changes are expected to result in expanded use of older first generation indandione compounds (FGARs; e.g., diphacinone, chlorophacinone). Recent acute oral and 7-day dietary diphacinone toxicity studies conducted in American kestrels (Falco sparverius) and Eastern screech-owls (Megascops asio) suggest that raptors are considerably more sensitive to FGARs than predicted by data developed with traditional avian wildlife test species (Northern bobwhite, Colinus virginianus and mallards, Anas platyrhynchos). Many studies have demonstrated that the toxicity of FGARs to target rodent pest species is more pronounced in a multi-day exposure scenario. Likewise, some data indicate that the toxicity of FGARs to non-target wildlife is greatly enhanced in a repetitive dietary exposure scenario. Regulatory agencies continue to require and use acute oral toxicity data (i.e., LD50 derived from single or multiple doses administered in a 24-hour period) as a significant component of their ecological risk assessments. While a valuable measure of toxicity, the LD50 can underestimate the toxicity of FGARs that can be more toxic when consumed over several days. Additional information examining the effects of varying the frequency and duration of FGAR exposure would improve risk assessments. Furthermore, sublethal FGAR responses (e.g., bleeding, coagulopathy, histopathological lesions) that may constitute biologically significant adverse effects are considered, but are given less weight in the overall risk assessment. Some of these adverse effects could affect survival of free-ranging birds in ways that would not be apparent in a controlled laboratory setting. Choice of test species, laboratory exposure regimens and toxicity endpoints, as well as better characterization of the probability of exposure in field situations, deserve further attention to more accurately assess the risk that FGARs pose to non-target wildlife.

RA22-4

Investigating the potential risk of secondary rodenticide poisoning to urban owls inhabiting and foraging in urban landscapes of the Lower Mainland, British Columbia, Canada

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Anticoagulant rodenticides are widely used to control pest rodents, but poisoning of non-target wildlife has been linked to these practices, including secondary poisoning of birds of prey, particularly owls. In this study, we investigate whether Barred owls (Strix varia), Great-horned owls (Bubo virginianus) and/or Barn owls (Tyto alba) inhabiting and foraging in predominantly urban landscapes of the Lower Mainland, British Columbia are at risk of consuming rodenticide-laden prey, such as rats and house mice. By conducting a pellet study, we found that urban Barred owls had the largest proportion of rats in their diet, with some individuals' diet consisting primarily of rats. Urban Great-horned owl pellets were also comprised mainly of rats, but there was a clear shift towards alternative prey base when urbanization within home ranges decreased. Field voles (Microtus townsendi) were the main prey item for Barn owls, regardless of the amount of urbanization within their home range. For all three species, consumption of rats and house mice appears to coincide with increased urbanization within home ranges. The shift in the diet of owls living in urbanized areas may potentially lead to an increased risk of secondary rodenticide poisoning. Radio telemetry was deployed to further investigate which landscape features urban Barn owls select as foraging habitat and whether they forage in proximity to buildings where rodenticide is applied. Urban Barn owls were found to predominantly forage in grass strips along highway interchanges and verges, and untended grass patches within the city. The majority of foraging was done within 100 m of commercial buildings where rodenticide had been applied. These findings will be discussed in conjunction with previous research done on rodenticide residues found in the livers of deceased owls and the current and historic sales of rodenticides in the Lower Mainland, British Columbia.

RA22-5

How the uses of anticoagulant rodenticides influence the distribution of their residues in rodent community?

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In Europe, the uses of anticoagulant rodenticides (AVKs) are regulated as biocides (Directive 98/8/EC) or as plant protection product (Directive 91/414/EE referred as pesticide uses hereafter). According to these uses, the active ingredients (a.i.) found in the commercial products and the quantities that are applied in the environment may be very different. Biocide uses of AVKs correspond to a large diversity of a.i. (8 molecules are homologated) which are applied around villages and habitations at relatively small quantities locally. Plant protection is authorized with 3 a.i. only and is commonly realized in eastern France with large amount of bromadiolone poisoned baits (up to 20 kg / ha) over vast areas (e.g., 12,000 ha in 2006) to control Water vole outbreaks. If large mortality events of rodent predators are generally associated to pesticide uses, secondary exposure of wildlife to biocide AVKs is now widely reported. Here, we aim to document the distribution of 8 AVKs in the rodent community according to the uses in eastern France. For each context of uses, 2 areas were selected and the localization and intensity of AVKs treatments were characterized as precisely as possible. Then, both target and non-target rodents were trapped in autumn up to 1 km from the place where AVKs treatments have been identified. The residues of the 8 AVKs authorized in Europe were measured in the liver and the whole body of 100 specimens selected in each area. Anticoagulant rodenticides were largely distributed in the rodent community of the treated areas whatever the type of uses. In the pesticide area, a high proportion of individuals in both target and non-target species were exposed to bromadiolone (45%) and the high levels of residues in some individuals (> 50,000 ppb in the liver for some Water voles and mice) may explain lethal poisoning of rodent predators. In biocide areas, median liver concentrations of all AVKs were 3.5 and 1.3 ppb in target and non-target species respectively, 25% of the specimens trapped exhibiting detectable residues of AVKs in the liver. This suggests that predators are frequently exposed to low doses of different AVKs but the impact of sublethal exposure of wildlife to rodenticides remains under question.

RA22-6

Risk mitigation measures for anticoagulants used as rodenticides in Sweden

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Anticoagulants used as rodenticides are non-selective, highly toxic substances. Second generation anticoagulants (SGARs) (bromadiolone, difenacoum, brodifacoum, flocoumafen and difethialone) are also persistent with extremely slow elimination from the body, and prone to accumulate in non-target species that consume poisoned rodents (secondary poisoning). They have characteristics which meet the criteria to be classified as potential PBT and potential vPvB substances. Furthermore, monitoring studies in several countries have shown high levels of second generation anticoagulants in predatory mammals, raptors and owls. Nevertheless, SGARs have been included in Annex I to Directive 98/8/EC because of their identified benefits for public health and the lack of established alternatives which are at the same time equally effective and less damaging to the environment.

If SGARs are to be used, extensive risk mitigation measures needs to be applied in order to reduce the risks for primary and secondary exposure for humans, non-target animals and the environment. The Swedish Chemicals Agency finds it appropriate to restrict authorisations of rodenticides containing SGARs to user category "class 1 - professional use with a specific permit". In combination with other risk mitigation measures, this is considered an appropriate way to reduce the risks yet allowing for effective rodent control.

RA23 - Wastewater effluent discharges: chemical characterisation and understanding potential risks in receiving waters

RA23A-1

The UKWIR Chemicals Investigation Programme

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Recent EU legislation in the field of water and the environment, in particular the Water Framework Directive (WFD), has important implications for the scope and nature of pollution control measures required to protect surface waters. Environmental Quality Standards (EQSs) have been set for substances that hitherto have not been subject to detailed monitoring or control. These standards have, in turn, generated a need for compliance assessment and, where necessary, the development of appropriate control measures. The UK Water Industry has responded to this challenge by collaborating with national environmental regulators to undertake a £25M programme of investigations of contaminants in wastewater, their fate and behaviour in wastewater treatment and their sources within urban sewer catchments. Effort is focussed on a range of over sixty contaminants, including priority substances regulated at European level, specific pollutants regulated at national level and a range of substances, including pharmaceuticals, of emerging importance. The project is intended to identify and prioritise substances that are likely to require future action under the Water Framework Directive. It also seeks to establish the sources of different substances and to determine the most effective forms of control, including measures not related to end of pipe treatment. This paper provides an overview of the chemicals investigation programme, describes its key outputs and provides examples of how the results of the programme have been used in order to prioritise proposed future measures to be implemented as part of the WFD. The relative performance of different wastewater treatment processes will be discussed in relation to the achievement of good chemical status for surface waters.

RA23A-2

Using target and non-target LC-MS/MS screening to characterise the presence of known and unknown micropollutants in wastewater

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Characterising the presence of organic micropollutants in wastewater effluents is fraught with challenges. The full assessment of the effectiveness of treatment options is often difficult as many organic micropollutants transform during the treatment process. Thus, a pure target screening approach may indicate that a compounds is no longer present following treatment, while the compound is still present but in a transformed state. We show here how this can be addressed using a combination of target and non-target screening approach on wastewater effluents. The program enviMass, developed in-house, was used to perform target and non-target screening of waste water effluents from around Switzerland. Between 97 and 111 of 376 target compounds were found and quantified using enviMass, with concentrations from low ng/L (lowest detection limit 5 ng/L) to µg/L levels. The number of transformation products detected as targets (over 10 per sample of a total of 30 TPs) indicates the significance of accounting for transformation processes in wastewater effluents and thus considering also "unknown"peaks when assessing samples. The number of non-target peaks varied greatly between the different plants, as did the presence of isotope peaks (providing some idea of peak identity) for positive and negative ionisations. Over 40 % of negative non-target peaks had sulfur present, attributed mainly to sulfonic acids. In contrast, many homologous series were detected in positive ionisation samples, generally resulting from peptides.
A comparison of peak intensities for target and non-target peaks revealed that of the top 20 peak intensities in negative mode, only 4 were target compounds. These were three artificial sweeteners (acesulfam, saccharin and cyclamate) and a pharmaceutical (diclofenac). The remaining non-target peaks are clearly a significant part of the sample, despite the comprehensive target list of environmentally relevant compounds selected for relevance to Swiss conditions and based on experience. Despite not knowing the identity of the non-target peaks, we show here that we can follow target compounds, transformation products and even non-target masses in wastewater effluents using an in-house software which is available for public use. The information extracted in the enviMass workflow can be used to quantify target and TPs as well as prioritise non-target compounds for identification and track these peaks in future monitoring programs.

RA23A-3

Occurrence of Pharmaceuticals on a sewage impacted section of a Mediterranean River (Llobregat, NE Spain) and their behaviour under different hydrological climate conditions

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Mediterranean rivers are characterized by high flow variability, strongly influenced by seasonal rainfall. In addition, the river receives effluent discharges of more than 55 WWTPs, and at some points especially at drought periods, the effluents may represent almost 100 % of the total flow of the river. When water scarcity periods occur, water flow and dilution capacity of the river is reduced. On the other hand, floods contribute to remobilization of pollutants from sediments. Consequently, the potential environmental risk of pollutants is expected to increase. Besides, due to continuing human pressure from extensive urban, industrial and agricultural activities, contamination levels in Mediterranean rivers are frequently higher than in other European river basins.
3,000 different pharmaceuticals (PhACs) are used in human medicine in the European Union. The main route of PhACs into the aquatic environment is excretion by humans and the direct disposal through domestic wastewater. Despite its previous treatment in WWTPs, depending on the efficiency and chemical properties of the compound are able to reach surface and ground waters. PhACs are widespread pollutants.Around 150 PhACs have been detected in the aquatic environment at levels in the ng/L range. However, little attention has been paid to behaviour of PhACs in surface waters.
In this context, this work aimed to trace presence of PhACs in sewage impacted surface waters and to determine relationships of levels of PhACs and flow under different hydrological conditions in order to gain information about effects of floods and droughts on these relationships. Sampling period (October 2009-July 2010) covered storm-flow events and river base-flow periods. Sampling sites were located downstream a dominant WWTP. A multiresidue analytical method based on LC-MS/MS after solid-phase extraction was used for sample analysis. 90 % of compounds targeted were present in at least one of the samples analysed. The most concentrated were at levels higher than 500 ng/L. Analgesics and antiinflammatories were the most ubiquitous and concentrated therapeutic group, determined in the range of 700-1700 ng/L. Target compounds were detected following an increasing gradient together with number of WWTPs distributed along the river section studied. Positive and negative correlations were observed pointing out the relevance of different hydrological phenomena like dilution effects or sediment re-suspension.

RA23A-4

PACs during wastewater treatment and in receiving waters - emerging issues

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Pharmacologically active compounds (PACs) are emerging contaminants found in surface waters at ppt levels. Thousands of PACs are approved for human/veterinary use, although only a very small percentage of these compounds have been studied in the environment. Some of the most commonly used PACs are sold in hundreds of tonnes/year in the UK alone. PACs enter the environment mainly through insufficiently treated sewage, waste effluents from manufacturing processes, runoff and sludge (if used as fertiliser or transported to landfill). They are ubiquitous and persistent (due to their continuous introduction into the environment) with synergistic properties. PACs have also been detected in drinking water, which poses a direct risk to humans and raises the issue of contaminated water sources. The necessity of research into PACs is widely acknowledged and the need for action to further improve our understanding of risks posed by PACs is often highlighted.
The aim of this presentation is to discuss efficiency of different wastewater treatment processes in the removal of PACs and to raise awareness of two important but underreported issues relating to the presence and fate of PACs in wastewater and their ecotoxicity. These are: (i) the possibility of under-reporting of the measured concentrations of certain PACs due to lack of routine measurement of these compounds in solids and (ii) possibility of a significant under or overestimation of toxicity of chiral PACs and incorrect environmental risk assessment due to lack of data on enantiomer-specific fate of these compounds during wastewater treatment and in the environment.

RA23A-5

Assessment of WWTPs efficiency to limit surface water pollution by illicit drugs

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Water contamination resulting from consumption of illicit drugs is a new concern for water management that must be considered, not only because of the social and public health aspects, but also in an environmental context, because of the contamination of surface waters by partially treatment efficiency of WasteWater Treatment Plants (WWTPs) discharging contaminated effluents.
It is now established that WWTPs influents contain illicit compounds at concentration included between some ng.L-1 to several µg.L-1 and leading to surface water pollution by WWTPs effluents incompletely treated. However, data are missing concerning illicit drug metabolites. In this way, we decided to study 18 drugs and metabolites and to compare WWTPs removal efficiency as a function of volume capacity and technologies of the treatment trains.

RA23A-6

Are the concentrations of micropollutants responsible for the reduction in wastewater toxicity for gammarids following the application of ozone?

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Micropollutants, which comprise among others pharmaceuticals and personal care products, enter the aquatic environment via secondary treated wastewater and are thus frequently detected in surface waters. To counteract the continuous release of these micropollutants, advanced treatment methods are currently under discussion. In this context the application of ozone is considered as an effective tool. However, its ecotoxicological implications are largely unknown. Therefore, the aquatic toxicity of secondary (=non-ozone) or ozone treated wastewater were assessed using the feeding rate of the leaf-shredding invertebrate Gammarus fossarum, which is known as a key-species in the ecosystem function of leaf litter breakdown. Two repetitive experiments resulted in significantly higher feeding rates for gammarids exposed to ozone compared to non-ozone treated wastewater sampled from a treatment plant equipped with a full-scale ozonation. While ozone was applied at the lab-scale, a further experiment confirmed the detoxification of wastewater from the same treatment plant following its treatment with ozone. Moreover, the deviations in the dissolved organic carbon profiles of ozone and non-ozone treated wastewater could be excluded as a driving factor, which required further experiments addressing this gap of knowledge. The two additional experiments displayed on the one hand a statically significant higher feeding rate of G. fossarum if exposed to ten-fold enriched eluates from solid phase extraction cartridges loaded with ozone compared to non-ozone treated wastewater. On the other hand, the mean feeding rate of gammarids exposed to non-ozone treated wastewater, which contained hardly any micropollutants (i.e. pharmaceuticals), was at the same level as wastewater from the same source but additionally treated with ozone. These results suggest the load (concentration) of micropollutants to trigger the effects displayed by the bioassay applied, while alterations in the organic matrix seem to be of minor importance. Hence, the feeding rate of G. fossarum appears to be a well-suited bioassay to indicate alterations in ecotoxicological properties of wastewater due to the application of advanced oxidation processes like ozonation.

RA23B-1

Do we need expensive advanced treatment of waste waters to prevent feminisation of wild fish?

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Oestrogenic contaminants are thought to be the major cause of feminisation (intersex) in wild fish populations. The major oestrogenic contaminants; oestrone (E1),17β-oestradiol (E2) and the contraceptive pill hormone 17α-ethinylestradiol (EE2), enter the aquatic environment via wastewater treatment works following human excretion. Widely used waste water treatment technologies are not completely effective at removing these steroids down to concentrations thought to be required to protect aquatic wildlife. A number of advanced tertiary treatment processes have therefore been proposed to reduce the concentrations of oestrogens entering the environment. It is imperative that we assess their efficacy: a) in terms of meeting proposed no-effect concentrations (PNEC) for steroid oestrogens and b) in mitigating the negative impacts of these chemicals on native fish populations.

This study assessed both steroid removal and intersex induction in a native UK fish species; the roach (Rutilus rutilus), maintained in a wastewater treatment works effluent following a variety of secondary, tertiary and advanced processes. Both adult and early life stage roach were exposed directly to either secondary activated sludge plant (ASP) effluent or to ASP effluent plus sand filtration (SF), chlorine dioxide (ClO_2), or granular activated charcoal (GAC) for a six month period. Analytical chemistry indicated that whilst ClO_2 and GAC treatments removed E1, E2 and EE2 most effectively, their concentrations still exceeded the suggested environmental quality standards (both individually and when combined) at multiple times during the course of the study. Notwithstanding the failure to remove steroid oestrogens down to proposed PNEC, both GAC and the substantially cheaper ASP plus SF were effective in reducing or preventing the occurrence of intersex in fish exposed to these effluents. With the exception of the control and GAC, intersex was induced in all other treatments, including the ClO_2 treatment, where it was seen at a comparable level to the ASP effluent, despite the fact that this effluent exhibited the lowest concentrations of steroid oestrogens. Our results highlight the possible danger of relying on chemical analyses alone to assess sewage treatment options for removing hazardous substances and indicate that nitrifying ASP treatment followed by SF may provide the most cost effective strategy for mitigating feminisation in wild fish caused by endocrine disrupting chemicals.

RA23B-2

Fate of oestrogens in a tertiary nitrifying sand filter

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The fate of hazardous compounds was assessed in a full-scale nitrifying sand filter as part of the chemical investigations programme, a UK national scheme instigated by the Water Industry and the Environment Agency to examine the fate of target compounds over a wide range of process units with the ultimate goal of developing adequate measures to meet the requirements of the Water Framework Directive.

Natural and synthetic estrogens are endocrine disrupting chemicals that can cause adverse effects on the sexual and reproductive systems in wildlife, fish and humans [1]. The nitrifying sand filter examined was a tertiary treatment process designed to remove wastewater solids and perform nitrification by specialized bacteria growing in a biofilm on the sand particles. The sand was continuously fluidized to control biomass growth and the accumulated solids removed by an airlift system [2].

From the 49 substances investigated a detailed overview on the fate of selected oestrogens: estrone, 17β estradiol and 17α-ethinylestradiol is provided. The wastewater quality, the sand filter performance and operation were also taken into consideration as well as the chemical-physical characteristics of the target compounds.

Several studies have reported a possible connection between nitrification and oestrogens removal [3], others have underlined the relevance of solids retention time [4] and the removal through sorption onto wastewater sludge [5]. The implications of using tertiary treatment processes for hazardous pollutants removal on energy and investment are also taken into account.

Final effluent concentrations were found to be in agreement with the values reported on literature [3]. Removals of E2, E1 and EE2 from the main stream were 89%, 78% and 21%, respectively. For proposed environmental quality standards E2 was always below the reference value of 1 ng/L; average concentration of E1 was below the reference 3 ng/L; but EE2 was was always above 0.1 ng/L.

Nitrifying sand filters remain a good candidate for a end of the line process for removal of oestrogens from wastewater although improvements are needed to meet environmental quality standards for 17α ethinylestradiol.

RA23B-3

The response of wild fish to Municipal Wastewater Effluent Exposures at sites in Canada

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The extent and implications of Municipal wastewater effluent (MWWE) of fish in the Canadian environment is currently poorly understood. The objective of this research was to examine the impact of MWWEs on the status of sentinel fish species at various levels of biological organization (cellular to community). Field studies conducted in the fall (2007) and spring (2009) in the Grand River watershed, Ontario, Canada, investigated the cumulative impact of two sewage discharges in an urban environment at reference sites upstream of the municipality of Waterloo, and at an intermediate site located between the two sewage treatment plant sites for Waterloo and Kitchener. Responses of wild fish [Rainbow Darter (Etheostoma caeruleum) and Greenside Darters (E. blennioides)] were assessed in terms of energy storage (condition factor), and energy utilization (reproduction: in vitro sex steroid production, gonadosomatic indices, and histology). Both sentinel species collected downstream of both discharges demonstrated greater growth (longer and heavier), however fish were not assimilating additional resources into energy storage (increased condition, liver somatic index). Exposed male darters had impaired capacity to produce androgens in vitro, lower GSI and altered sperm cell staging. Exposed female fish also had impaired capacity to produce estrogens in vitro. Intersex in male darters collected during the fall downstream of both sewage discharges studied while upstream agricultural and urban reference sites demonstrated low levels of intersex. Pre-spawning darters demonstrated dramatically higher incidence of intersex at both the near-field and far-field exposure sites and coincide with reductions in gonadosomatic indices and steroids. The fish communities downstream of these outfalls demonstrated differences in abundance, diversity, and species composition when compared to the fish community upstream or further downstream of the points of effluent discharge. Changes in the species composition downstream of the outfalls occurred with larger more mobile, tolerant fish species such as suckers and sunfish becoming more common. The potential exists for a cumulative impact of multiple outfalls of treated wastewater effluents as changes were more pronounced downstream of the second sewage discharge. This research demonstrates the potential cumulative effects of MWWE discharges in Canadian rivers on fish responses at various levels of biological organization.

RA23B-4

Reducing and monitoring toxicity in an industrial effluent, using a regulatory approach

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Between 1997 and 2000 the UK government started to try to regulate complex effluents using Direct Toxicity Assessment (DTA). Sites were selected, effluents screened and then ranked for further investigation. This was followed by characterisation, risk assessment, toxicity reduction efforts and monitoring.

In this case study we explore a data set spanning 8 years where we applied these processes for an industrial chemical company, resulting in a collaboration that significantly reduced the final effluent acute toxicity.

Effluents were tested using *Tisbe battaglia* and *Skeletonema costatum* bioassays. High toxicity was identified and it was decided that the effluent needed moderating before it could be allowed to be disposed of to river. The most toxic samples were analysed and Phenol and formaldehyde were identified as key contaminants. Their contribution to the overall toxicity was calculated using a toxic units approach. Assays were preformed according to the UK EAs Standard Committee of Analysts methods and were carried out every month from 2003 until the present. The most toxic samples taken through the industrial process were analysed for phenol and fomaldehyde and found to have high concentrations in the 1000's mg/l range. A new piece of equipment was introduced to scrub these specific chemicals from the effluent before it was discharged to the environment.

Following the introduction of the new plant in 2006, detectable toxicity in the two bioassays dropped significantly and has remained low, apart from one unexplained peak in 2008.

This shows the success of the DTA approach and the potential it has to lead to solutions that work for industry and the regulators in reducing toxic inputs to the environment.

RA23B-5

Evaluating advanced treatment of hospital wastewater

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This study aims to evaluate the importance of hospitals as point sources of pharmaceuticals into the environment and to propose possible measured to minimize the pharmaceutical input. For that purpose, a pilot-scale wastewater treatment membrane bioreactor (MBR) was operated at a Swiss cantonal hospital over one year. Part of the

MBR permeate was further treated either by powdered activated carbon (PAC), ozone, or photocatalysis (UV/TiO2). Employing robust sampling strategy and quantifying over fifty highly consumed pharmaceuticals by online SPE-LC-MS/MS provides robust and reliable results. Measurements of species-specific resistance determinants as well as multi-resistant Pseudomonas aeruginosa have shown that hospitals release high amounts of antibiotic resistant and multi-resistant bacteria to the environment. Hospitals are also major contributors to the load of contrast media, some antiinfectives and anesthetics in the environment. Decentralized hospital wastewater treatment is techniqually possible and ozonation as well as PAC treatment can be recommended as techniques to reduce pharmaceutical load as well as ecotoxicological effects. For most pharmaceuticals high elimination rates were achieved with both treatments; lowest eliminations were observed for the contrast media diatrizoate and ioxitalamic acid. Elimination efficiencies observed in hospital wastewater treatment were similar to the ones in municipal wastewater treatment. Results will be used to support the legal decision weather or not decentralized hospital wastewater treatment would be an option for Switzerland.

RA23B-6

An examination of the toxic properties of water extracts in the vicinity of an oil sand extraction site

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The industrial extraction of oil sands (OS) in northern Alberta, Canada, has raised concern about the water quality of the nearby Athabasca River. The purpose of this work was to examine the toxic properties of various water extracts on Oncorhynchus mykiss trout hepatocytes. The water samples were fractionated on a reverse-phase C18 cartridge and the levels of light-, medium- and heavy-weight polycyclic aromatic hydrocarbons (PAHs) were determined by fluorescence spectroscopy. Primary cultures of trout hepatocytes were exposed for 48 h at 15oC to increasing concentrations of the C18 fraction corresponding to 0.02, 0.1, 0.5 and 2.5X concentrations from upstream/downstream sites in the Athabasca River, groundwater samples, OS tailings and interceptor well-water samples. Changes in cell membrane permeability, activity of phase I and phase II biotransformation enzymes (cytochrome P4501A and glutathione S-transferase activities), oxidative damage (lipid peroxidation LPO) and genotoxicity (single and double DNA strand breaks) were monitored in post-exposure cells. The water samples produced minor changes in membrane permeability but did increase all the above endpoints at thresholds of between 0.02 and 0.1X the water concentration. The most responsive biomarker was DNA damage but it also offered the least discrimination among sites. LPO was stronger at sites downstream of the industrial operations compared to upstream sites. A decision tree analysis was performed to formulate a set of rules by which to identify the distinctive properties of each type of water sample. The analysis revealed that OS tailings and interceptor waters were characterized by an increased concentration in light PAHs (> 42 µg/L) and this fraction represented more than 85% of the total PAHs. These samples also inhibited GST activity, which could compromise the elimination of genotoxic PAHs present in the system. An analysis of groundwater samples revealed a contamination pattern similar to that for OS tailings. There is a need for more research into specific biomarkers of toxicity from OS tailings compounds such as naphthenic acids, light PAHs among others, which are a characteristic fingerprint of OS extraction activities.

EC01P - Advances in passive sampling and dosing techniques

MO 001
Calibration and field deployment of five integrative samplers for the monitoring of indicator and dioxin-like PCB (ECLIPSE project)
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Various integrative samplers, at different stages of development, are now available to estimate time-weighted average (TWA) concentrations of freely dissolved hydrophobic contaminants in aquatic environments. The ECLIPSE project (2009-2011, coord. C Miège, Irstea) involves 5 laboratories and aims to calibrate and compare 5 different integrative samplers for the monitoring of indicator and dioxin-like PCB in water: semi-permeable membrane device (SPMD, studied by Irstea), low-density polyethylene strip (LDPE, Ifremer), silicone rubber (SRPS, Deltares), Chemcatcher® (BRGM) and continuous-flow integrative sampler (CFIS, LABAQUA).
The first step of the project was the simultaneous calibration of these samplers under laboratory conditions. During summer 2009, samplers were exposed under constant agitation and temperature in a stainless steel tank filled with 200 L of PCB contaminated water. A constant PCB concentration of about 1 ng/L was achieved by immersing a large amount of silicone rubber sheets [Rusina 2010] spiked with indicator and dioxin-like PCB. Prior to deployment, samplers were spiked with Performance Reference Compounds (PRC) and exposure durations ranged from 1 day to 3 months. After exposure, processing and analysis, samplers were compared in terms of sampling rate, linear uptake phase duration, repeatability and accuracy of calculated TWA concentration.
The second step of the ECLIPSE project was the deployment and comparison of these samplers in real aquatic environments. In summer and autumn 2010, and in spring 2011, three field campaigns were carried out along the Rhône River and near the lake Le Bourget (France), known to be contaminated by PCB. Using appropriate cages, canisters and holders, studied samplers were exposed simultaneously at an approximate depth of 1 m during 1, 2, 3 and 4 weeks with duplicates and/or triplicates. These field campaigns allowed to compare in-situ ease of use and robustness of the five integrative samplers in addition to repeatability of sampling and TWA concentration estimate.

MO 002
An international collaborative study on the use of passive samplers in monitoring of emerging pollutants
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It is now being recognised that passive samplers can play a valuable role in monitoring water quality within a legislative framework such as the European Union's Water Framework Directive (WFD). The time-integrated data from these devices can be used to complement chemical monitoring of priority and emerging contaminants which are difficult to analyse by conventional conventional spot or bottle sampling methods, and to improve risk assessment of chemical pollution. In order to increase the acceptance of passive sampling technology amongst end users and to gain further information about the robustness of the calibration and analytical steps, several inter-laboratory field studies have recently been performed in Europe. Such trials are essential to further validate this sampling principle and to increase the confidence of the technological approach for end users. An inter-laboratory study on the use of passive samplers for the monitoring of emerging pollutants was organised in 2011 by the NORMAN association (Network of reference laboratories for monitoring emerging environmental pollutants; www.norman-network.net) together with the European DG Joint Research Centre to support the Common Implementation Strategy of the WFD. Thirty academic, commercial and regulatory laboratories participated in the passive sampler comparison exercise and each was allowed to select their own sampler design. All the different devices were exposed at a single sampling site to treated waste water from a large municipal treatment plant. In addition, for each target analyte class the organisers deployed in parallel, multiple samplers of a single type which were subsequently distributed to the participants for analysis. This allowed an evaluation of the contribution of the different analytical laboratory procedures to the data variability. The results obtained allow an evaluation of the potential of different passive sampling methods for monitoring selected emerging organic pollutants (pharmaceuticals, polar pesticides, steroid hormones, fluorinated surfactants, triclosan, bisphenol A and brominated flame retardants). The exercise was a great learning experience for organizers and participants. The results will be used to inform EU Member States about the potential application of passive sampling methods for monitoring these compounds within the framework of the WFD.

MO 003
Method for passive sampling of TBT in surface waters using silicone rubber - field application
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Maximum permissible concentrations of tributyltin (TBT) in the aqueous phase are lower then the limits of detection for common analytical methods. Passive sampling can accumulate contaminants from large volumes of water and was suggested as a method for the determination of TBT in surface waters. Analytical aspects of passive sampling using silicone rubber and the determination of parameters to convert sampler uptake into aqueous phase concentrations, i.e. sampler-water partition coefficients as well as diffusion coefficients in sampler material were investigated. Sampler water partition coefficients were higher then expected from octanol water partition coefficients and suffered from the presence of particulate matter. Diffusion coefficients for mono and di-substituted organotin compounds were low, such that diffusion in the sampler is partly controlling the uptake. This requires that for calculation of aqueous phase concentrations both water boundary layer transport and diffusion in the sampler needs to be taken into account. Several field trials were executed. Samplers were deployed for 6-8 weeks, in harbor areas in the Netherlands and at 6 sites in the UK, on a transect from the tidal limit of the Thames down to the Outer Estuary. This poster describes the method developed as well as results of the field and evaluates the applicability of silicon rubber as a suitable passive sampler for butyltin compounds.

MO 004
Comparison of uptake rates of pharmaceuticals and organophosphate flame retardants in a range of passive samplers
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Passive samplers have been widely used to a range of contaminants. In this study, a range of passive samplers (Chemcatcher (polar), Chemcatcher (non-polar), POCIS, SPMD and PDMS (silicon rubber)) were assessed in a laboratory study. The samplers were deployed in a tank with a continuous flow of water from a header tank, which was set at a rate to allow complete replacement of the water in 30 minutes. Into the header tank, a known concentration of chemical was dosed. Compounds investigated were pharmaceuticals and Organophosphate flame retardants.
The purpose of this tank test is to determine suitability of each of the four samplers in the analysis of these compounds, and to establish sampling rates for the compounds of interest.
The water replenishment meant that we could be confident that any removal of the contaminant by samplers was not sufficient to significantly reduce the concentration of that contaminant in the water phase (meaning that the concentration could be assumed to be constant). Samplers were removed from the tank weekly and the study was terminated after four weeks exposure. Samplers were then extracted and the extracts analysed for the spiked compounds. Relative uptake rates of various compounds to different samplers were established.

MO 006
Simultaneous quantitative analysis of pesticides including Phenoxy-Acids in surface water using UPLC-MS/MS with direct injection
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LC/MS/MS is widely used, in combination with solid phase extraction techniques, to achieve the very low detection levels (low ppt range) needed for the monitoring of pesticides and other pollutants like pharmaceutical drugs in surface and drinking water. Various approaches are possible, depending on the performances on the MS instrument, on the needed sensitivity and on the nature of the sample (drinking or surface water). SPE is usually done off-line, starting from a large volume of water (up to 500 ml to 1 l), with associated drawbacks (long protocols, transportation of the samples, cost). Preconcentration can also be done automatically on-line, with different draw backs (recoveries for compounds from different classes, robustness of the method for surface water). The evolution of HPLC to Ultra Performance LC (UPLC) and new generation of tandem-quadrupole mass spectrometer bring additional possibilities. The analysis of most pesticides is now possible at low ppt by direct injection.
The LC-MS/MS method that we present has been developed for the quantitative analysis of pesticides including phenoxy-acids. The chromatographic separation is done using a Waters ACQUITY UPLC system. The MS detector is a Waters Xevo TQ-S tandem quadruple, operated in ESI mode, with fast polarity switching. For each analyte, the most intense MRM transition was quantified and reported. This method allows the analysis of more than 4 samples per hour. Surface water samples were filtrated, spiked with the internal standard (deuterated compounds) before injection (250µl).
The analysis of more than 25 basic pesticides residues and of phenoxy-acids was done simultaneously in less than 15 minutes, injection to injection. This method revealed an excellent linearity across the studied range (5-500 ppt) and an excellent repeatability with RSDs typically lower than 2% over 10 injections at mid concentration. Limits of detection range from 5 ppt for the less sensitive compound (MCPB), to below 0,02 ppt for the most sensitive compound (Carbendazim). Despite the very minimum sample

preparation, the UPLC column lifetime was several thousand injections.This methods brings a significant gain in time (acidic and basic compounds in a single injection), and in cost (sample preparation is limited to filtration). Possible developments on this method is the inclusion of other molecules, including PPCP (Pharmaceutical and Personal Care Products).

MO 007
Monitoring trials for detection of ionic herbicide residues in water using passive samplers
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Passive samplers for routine monitoring of pesticide residues in irrigation channels and rivers have already been developed for a number of hydrophobic compounds. However, some polar, hydrophilic ionic herbicides such as glyphosate and amitrole are either not retained in such samplers or are difficult to dislodge from membranes specifically designed to capture polar compounds. Development of new passive sampling devices for such herbicides required first the development of a suitable analytical method for detection of their residual amounts in environmental samples. An electro-chemical detector fitted to a HPLC system detected with accuracy and sensitivity these and other common herbicides found in agricultural waters (1). Secondly, SDB-RPS Empore® disk membranes were found to perform best for accumulating amitrole, and were chosen for calibrating a passive sampling device containing these membranes under flow-through laboratory conditions. Whilst SDB-XC Empore® disk membranes could be used to retain and extract glyphosate from spiked water samples filtered through them, this membrane was unable to accumulate this herbicide in a flow-through system. Instead, glyphosate accumulated in a passive sampler device consisting of Amberlite® IRA67 resin pre-washed with 1M NaCl, dried and then packed in nylon mesh bags (240 micron) that were subsequently tested under the same flow-through laboratory conditions. Both herbicides could be extracted from their respective samplers by the same extraction method using 10 mM NaOH, which facilitated the processing and analysis of the herbicides taken up by the passive samplers. A field trial to test the performance of both types of sampling devices when deployed in agricultural irrigation channels was carried out. Results from the field trials are still under way, and will be presented to show whether the mean time-integrated pesticide concentrations taken up by the passive samplers compare with the cumulative mean water concentrations calculated from daily extractions using the Empore disk membranes.

(1) Sánchez-Bayo, F., Hyne, R.V. and Desseille, K.L. (2010) An amperometric method for the detection of amitrole, glyphosate and its aminomethyl-phosphonic acid metabolite in environmental waters using passive samplers. Anal. Chim. Acta 675(2): 125-131.

MO 008
Ionic compounds and SPE materials - What do you have to bear in mind?
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A wide variety of environmental compounds of concern, *e.g.* pharmaceuticals or illicit drugs, are acids or bases that may be predominantly present as charged species in drinking water sources. These charged micro pollutants happen to exists in the environment in large numbers due to anthropogenic activities. Many of these compounds have a high affinity towards water and sampling is often difficult due to the fact that many commonly employed sorption materials are designed to adsorb neutral compounds. Therefore, sorption materials allowing coulomb interaction are often used to enable sampling of these compounds. Detailed knowledge on their sorption behaviour, however, is sparse, especially concerning passive sampling in environmental monitoring. The exact influence of both the charged and the neutral moiety on the sorption behaviour is not yet well-investigated. The influence of various inorganic ions (e.g. Ca^{2+}, Cl^{-}), that are commonly present in water, on the sorption affinity is just as little understood. Competition for the charged sorption sites can be expected and consequently a decrease in sorption affinity.
For this research sorption coefficients in different water matrices for various charged compounds, such as pharmaceuticals and ionic liquids, were derived from measured retention times on columns filled with ion exchangers and SiC as inert support material. The results show that apolar interaction of charged compounds with the sorption material is an important factor regarding sorption affinity. The more pronounced the apolar moiety is, the higher the sorption coefficients. Equally important is the influence of various inorganic salts in the water phase. This study shows that for *e.g.* metformin changing from Ca^{2+} to Na^{+} the sorption coefficients on a cation exchanger rise by one order of magnitude.
These results help to evaluate if the employment of passive samplers for a compound is useful under certain conditions. It becomes clear that sampling in e.g. Ca^{2+} rich water is more challenging than in Na^{+} containing water and that small organic ions with a lack of apolar moieties are difficult to concentrate on a passive sampling materials so far.

MO 009
Development of novel monitoring, analytical chemistry and modelling methods for improving the ecological risk assessment of radioactive caesium in the aquatic environment in East Japan
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Pollution by radiocaesium of the area surrounding the Fukushima Daiichi nuclear power plant is expected to be persistent for many decades in surface waters, soil, foodstuffs and in aquatic and terrestrial organisms. Following a nuclear accident, it is crucial to accurately measure, monitor, and model concentrations of radioactive caesium in the environment. Due to widespread dispersion of this radioelement across Japan, low-cost, simple (but accurate) monitoring methods are needed and these should be easy to interface with existing instrumental analytical techniques.
We aim to develop a passive sampling device to measure TWA concentrations of radioactive caesium in aquatic environments in East Japan based on the Chemcatcher®. No passive sampler currently exists for measuring radioactive caesium. Chemcatcher® was developed and patented by the Portsmouth University team (UoP). It is proposed that UoP models be adapted to predict long-term contamination of freshwater ecosystems in Japan using Chemcatcher® sampling data.
We are also developing new analytical procedure of radioactive caesium in aquatic environments including surface water, sediment, aquatic biota, which will take much shorter time to analyze the concentration. This presentation will show novel monitoring methods, analytical procedure and results from field monitoring for radioactive caesium in aquatic environments.

MO 010
Seasonal monitoring of organic UV filters and UV light stabilizers in coral reef water and beach water by passive samplers
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A great deal of attention has been directed to the ecological risk associated with organic UV filters and UV light stabilizers in aquatic environment, especially in beaches and coral reefs. Recreational activities such as swimming may be one of major direct inputs of organic UV filters into beaches and coral reefs. Moreover coral reefs near estuaries could be affected by river water which often contains organic UV filters and UV light stabilizers originated from human activities.
Seasonal monitoring of eight organic UV filters and 10 UV light stabilizers in coral reef water and beach water was conducted in Okinawa from March to September 2011. Passive sampling method was adopted using TRIMPs in order to reveal seasonal variation of 18 analytes in reef waters. The Chemcatcher® was also deployed for the measurement of preservatives from cosmetics. Grab samples were also collected monthly in beach water.
Passive sampling in coral reefs revealed more than 100 times higher concentration of octyl salycilate, homosalate, benzophenone-3, EHMC and octocrylene in summer than in winter. They were also observed at much higher concentration in beach waters in summer. These results indicated that these compounds released from recreational activities, especially swimming, could have a potential ecological risk to coral reef ecosystems.

MO 011
Calibration data for Polar organic chemical integrative samplers (POCIS)
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Polar Organic Chemical Integrative Samplers (POCIS) have been originally developed for sampling polar compounds from the aquatic phase. POCIS consist of an adsorbent which is enclosed by a polyethersulfone membrane. A crucial step in order to utilize POCIS for the quantitative determination of aqueous concentrations is to determine uptake rates, which is usually done in the laboratory in separate calibration experiments.
Calibration data based on own experiments and uptake rates retrieved from literature have been collected in a database. The data set comprises more than 300 single values of uptake rates. This contribution will compare results from calibration experiments and look for relationships between the compound's properties and its uptake rate, with the final goal to predict uptake rates by properties or structures of the targeted compounds. The influence of varying environmental conditions during the calibration process will be discussed, and uncertainties in uptake rates will be examined.

MO 012
In-situ validation of 3 PRCs and calibration of 14 pharmaceuticals and 20 endocrine disruptors on the polar C18 Chemcatcher
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In response to the growth of organic pollutants identified in surface water many multi-residue analytical methods have been developed to quantify multi-families of emerging pollutants in water. Many strategies include enrichment steps for water samplings due to very low levels of pollution [1]. Recently, sampling systems more realistic of

environmental exposure have been designed to get time weighted average (TWA) concentrations of those xenobiotics. Those passive samplers enable further investigation for toxicological effects on the environment or populations of such mixture and concentrations.
The polar C18 Chemcatcher has been evaluated for the monitoring of multi-families of Endocrine Disruptors and Pharmaceuticals. First C18 Chemcatcher with PES diffusion membrane have been rigorously calibrated for 34 emerging organic pollutants. Secondly a PRC approach (Performance Reference Compounds) has been investigated [2]. Samplers have been exposed for 28 days in a 50L flow through microcosm for the adsorption study and spiked samplers with tap water for the desorption experiment. Finally samplers were exposed for 3, 7 and 14 days in surface water in two rivers near Lyon.
All the 34 calibrated molecules showed good correlation to first order accumulation with half time of equilibrium above 14 days for most of those molecules. Good linear relationships were obtained (R^2 from 0.90 to 0.99) for 7 to 21 days on the C18 Chemcatcher. Sampling rates were calculated between 0.005 and 0.16 L/d. 3 molecules showed accumulation and desorption consistent with first order kinetics with similar half time of equilibrium and thus verifying all criteria for their use as PRCs. Exposure campaign allowed to validate PRCs comparing TWA concentrations obtained from passive samplers to average concentrations detected in grab sampling analyzed by online-SPE-LC-MS/MS method.

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MO 013
Comparative analysis of pesticide monitoring via traditional surface water sampling and Chemcatcherβ passive samplers
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Pesticide monitoring in European surface waters is regulated by the Water Framework Directive (WFD) establishing environmental quality standards (EQS) for the good chemical status of water bodies. EQS monitoring is based on analyses of pesticides in water samples. WFD requires at least monthly sampling for assessment of maximum annual average concentrations. Due to the high temporal variation of pesticide use and leaching and discharge conditions in running waters, such robust monitoring approach may fail to detect pesticides, especially peak concentrations. We compared traditional water sampling results to pesticide concentrations detected with Chemcatcher® passive samplers in a large peatland river Kyrönjoki and its small tributary Lehmäjoki. The Chemcatchers® were deployed in four separate trials on both sites for two weeks time period during 21 Jun - 30 Aug. The traditional water samples were analysed twice a month in Lehmäjoki and monthly in Kyröjoki.
The number of compounds found in Chemcatchers® was 32, while in water samples 27 pesticides were detected but only 15 of them were quantified. High concentrations of some pesticides not detected in traditional water sampling were found with Chemcatchers®.
The preliminary results clearly indicate that measurement of pesticides from water samples is prone to failures to detect their actual presence in water bodies. Passive sampling with Chemcatcher® should also be compared simultaneously with other methods which have commonly been used earlier in monitoring organic pollutants, like natural biota, sediments and bioaccumulation using mussels.

MO 014
Estimating herbicide contamination in flowing waters using passive sampling (POCIS) coupled with an algal bioassay
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Herbicide contamination of water bodies occurs mainly through run-off and leaching from agricultural fields as well as through spray drift. In-stream concentrations of herbicides may be highly variable with peak concentrations occurring in pulses following rain events. Traditional grab sampling is of limited value because this point of time estimate of herbicide contamination fails to accurately integrate pulses in concentration. Passive sampling techniques have the potential to eliminate this problem by providing time weighted average concentrations. Of the existing passive sampling technologies available, polar organic chemical integrative samplers (POCIS) show the most promise for assessing herbicide contamination and may also be used to measure concentrations of a wide variety of polar organic contaminants. In spring and summer 2010, POCIS were deployed at sites located throughout the South Nation River watershed, an agricultural watershed in Ontario, Canada. Three POCIS per site were deployed for two 28-day periods. One litre grab samples were taken at the beginning and end of each deployment to compare passive sampling with grab sampling. Grab samples were filtered, spiked with 1 µg/L deuterated atrazine and contaminants concentrated on 500 mg Oasis® HLB cartridges. Extracts were analyzed for atrazine via LC/MS/MS. Relative toxicity of the extracts was compared by exposing the green alga *Pseudokircheriella subcapitata* to extracts using an existing bioassay method. One issue with passive sampling in general is that daily sampling rates are influenced by a number of different factors such as temperature, stream velocity and biofouling. A calibration study to estimate how widely sampling rates vary in streams with different chemical and physical properties was conducted in fall 2010 and summer 2011 at six different streams. POCIS were spiked with 5 µg deuterated desisopropyl atrazine (a metabolite with high fugacity). Both the fall and summer experiments were conducted over 28-days, with three POCIS removed from each field site weekly. Comparisons between grab sampling and passive sampling will be discussed, along with the feasibility of using desisopropyl atrazine as a performance reference compound. In addition, the merits of using of passive sampling coupled with an algal bioassay to assess herbicide contamination and direct further monitoring will be discussed.

MO 015
Performance of three passive samplers and sediment for detecting agrochemicals
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Due to intensive agricultural land use, Victorian waterways (South-East Australia) may contain a large number of agrochemicals (pesticides), some of which may prove directly toxic to organisms living therein, while others may elicit more subtle effects. Managing the effects of such contaminants ultimately requires information on effluent toxicity and chemical concentrations. Time integrative sampling of waterways with passive samplers (or passive sampling) is a technique which facilitates cost-effective monitoring of chemicals found at very low concentration in a range of aquatic ecosystems. In our presentation, we present the results of one of the most comprehensive examinations of the input of pesticides in surface waters encompassing the measurement of 84 pesticides in sediments and three different passive sampling devices in 24 streams over a period of 5 month
Of the three passive samplers used, in short there were 28 individual pesticides observed amongst the 319 detections in the SDB-XC disk extracts. The most commonly observed chemicals (n>10) were simazine, myclobutanil, pirimicarb, pyrimethanil, imidacloprid, hexazinone, metalaxyl, atrazine and carbaryl. There were 27 individual pesticides observed amongst the 319 detections in passive TRIMP sampler solvents, with the most commonly observed chemicals (n>10) being dieldrin, trifloxystrobin, pyrimethanil, and pirimicarb. Only seven agrochemicals were observed in extracts, although these observations included two chemicals not observed in the TRIMP or SDB-XC disk extracts, namely malathion and propyzamide, In natural sediment 34 pesticides were observed amidst a total of 266 detections, with the most commonly observed chemicals (n>10) being p,p-DDE, simazine, myclobutanil, pyrimethanil, dieldrin and spinosad.
This study confirmed that passive samplers appear most suited to investigation of non-polar compounds, with the Chemcatcher system utilizing an SDB-XC disk most suitable for moderately polar pesticides. Passive samplers with receiving phases of different thickness such as the silicone rubber passive samplers may give valuable insights into uptake kinetics of compounds. Sediments collected a wide range of chemicals. Overall, sediments are probably most suitable to monitor a wide range of hydrophobic compounds, while passive samplers can complement important information on exposure kinetics, water concentrations and hydrophilic compounds.

MO 016
Analysis of Polar organic pollutans in the environment by means of continuous flow integrative sampler (CFIS)
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In order to obtain a good ecological state in body of water it is necessary to implant new continuous sampling system as passive or integrative samplers. In this way, the WFD and UNE-NORMES are introducing and recommending the use of new methodologies.
However, the range of possibilities for the development of new devices is relatively restricted by the theoretical principles governing passive sampling. In most of the actual passive samplers, the variation in the uptake values which result from the variations in turbulence can generate important problems in determining accurately time weighted average concentrations obtained from sampling rates calculated from tests under laboratory conditions. In samplers which are based on sorbents, the problem has been partially resolved by using performance reference compounds (PRCs). Nevertheless, the problems of turbulence vs. sampling rate are still the main sticking point of passive samplers of polar compounds in general, with sorbents governed by adsorption principles. In these cases the Rs must be estimated with a theoretical approximation. Apart of from, the Rs have been influenced by temperature and a control of this parameter is crucial in order to obtain a accurate time weighted average concentrations.
Another important limitation of passive sampling techniques resides in the fact that only the dissolved fraction (bio available fraction) is sampled. The suspended solid and colloid fraction information is not given as required in different legislations.
In this work we present the results obtained with a new device (Continuous Flow Integrative Sample (CFIS) for the time weighted average monitoring of water quality has been present. The results obtained in some different campaigns (waste water, river water and marine water) in different sampling points:
- Waste water. WWTD after secondary treatment.
- Surface water. Ebro river.
- Marine water. Soller Port.
The results obtained with CFIS have been compared with spot samples

MO 017

Impact of biofouling on DGT measurements in water

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The technique of diffusive gradient in thin film (DGT) is commonly used to assess metal contamination in natural waters. In this study, we assess the effect of biofouling on DGT measured labile concentrations in water and investigate whether an additional nuclepore polycarbonate membrane on the surface of DGT devices can limit biofilm growth. Simultaneous field deployments of DGT equipped with and without the additional membrane in a canal receiving wastewater were compared. The effect of the biofilm was also assessed in controlled laboratory experiments, completed by the experimental determination of several metals diffusion coefficients in the hydrogel and membrane systems. Biofilms effect was problematic only from the tenth day of accumulation. Accumulation of some elements is highly biased by the presence of a thick biofilm (Zn, Ni, Cd). It improved the quantification of Cd and Ni, but adversely affects the quantification of Cr and Co. A kinetic model is proposed to explain biofilm role on the DGT measurement. Depending on the metals of interest, it is possible to limit bias due to biofilms by using an additional polycarbonate membrane.

MO 018

Estimation of water concentrations of PAH, PCB and OCP by using semi permeable membrane devices with performance reference compounds

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Among the passive samplers, lipid containing semipermeable membrane devices (SPMDs) have been most commonly utilized in several matrices of the environment such as water, sediment and air. Lipophylic environmental contaminants have been frequently identified in several compartments of the global ecosystems. In this study, the water sampling rates and concentrations of polycyclic aromatic hydrocarbons (PAH), polychlorinated biphenyls (PCB) and OCP organochlorine pesticides were estimated by using SPMDs spiked with performace reference compounds (PRCs) at five sampling sites in the Istanbul Strait and Marmara Sea. Water sampling rates (Rs) for PAHs calculated by using the sampling rates of selected PRCs were negatively correlated to the Kow values of the corresponding PAHs. Generally, the sampling rates for all compounds after 7 days of deployment were similar indicating the similar conditions during the exposure period. The differences in sampling rates were more pronounced after 21 days of exposure. Water concentrations (Cw) of total PAHs vary depending on the Rs values used during the calculations and range from 69-193 pg/L and 47-211 pg/L and for Rs1 and Rs2 respectively for 7 days of exposure. Napthalene, Fluorene, Phenanthrene, Pyrene and Fluoranthene were the dominant PAHs in seawater. Estimated PCB water concentrations by using Rs1 and Rs2 values were very similar and found between nd - 2.17 pg/L and between 0.28 pg/L -2.4 pg/L respectively. According to the estimations, indicator PCBs were the dominant compounds in sea water and most of the non-ortho and mono-ortho PCBs were absent in the water phase. Among OCPs, HCH and DDT derivatives were dominant at all stations.

MO 019

Vertical fluxes of Polycyclic Aromatic Hydrocarbons in the Pelegrino Field (Southeastern Brazilian Shelf): preliminary results

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Pelegrino Field is a region located at 23°20'S - 41°12'W on Southeastern Brazilian Shelf that recently has being explored for petroleum resources. Therefore, the adjacent marine environment may be impacted by the introduction of material from the drilling activities. Polycyclic aromatic hydrocarbons (PAHs) are an important proxy for the identification of this impact, because they are present in petroleum and its products, indicating introduction of these materials in the marine environment. Sediment traps are a passive sampling tool used to monitor the impact caused by drilling activities. The aim of this study is to evaluate the amounts and fluxes of PAHs on Pelegrino field. Settling suspended matter (SSM) were sampled using two sediment traps (S1 - 23°18'S, 41°13'W; and S3 - 23°18'S, 41°12'W) equipped with 20 cups filled with mercury chloride ($HgCl_2$) to prevent organic matter bacterial degradation. The sediment trap area was 0.650 m² and sampling interval was three days. PAHs concentrations were determined by gas chromatography coupled to mass spectrometer detector (GC/MS). Overall, PAHs concentrations suggest a low level of contamination, since levels were lower than 250 ng g^{-1}. PAHs amounts show no difference between S1 and S3. Total PAHs (parental and alkylated PAHs) ranged from 12.2 to 687 ng g^{-1}, with similar average for both sediment traps (S1 223 ng g^{-1}; S3 199 ng g^{-1}). There is also no difference between amounts and proportions of low molecular weight (LMW) and high molecular weight (HMH) PAHs. S1 presented on average 48.9% of LMW and 51.1% of HMW, while S3 shown 42.2% of LMW and 57.8% of HMW. It suggests a mixture of PAHs derived from both petrogenic and pyrolytic sources on the SSM, which may results from both drilling and sailing activities in the area. SSM vertical flux shows a great difference between S1 and S3. S1 presented average flux of 600 mg m^{-2} d^{-1}, whereas S3 showed much higher values, 2881 mg m^{-2} d^{-1}. This was reflected on total PAHs fluxes. S1 ranged from 10.4 to 317 ng m^{-2} d^{-1}, while S3 ranged from 43.2 to 2400 ng m^{-2} d^{-1}. Although PAHs levels were similar between S1 and S3, vertical fluxes showed that S3 area exports more PAHs through the water column suggesting that S3 area is being more impact by drilling activities than S1.

MO 020

Evaluation of different passive samplers to predict uptake of polycyclic aromatic hydrocarbons by crop plants

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Polycyclic aromatic hydrocarbons (PAHs) belong to a class of hydrophobic organic pollutants, produced during the incomplete combustion or pyrolysis of organic materials from primarily anthropogenic sources such as fossil fuels and agricultural waste. The fate of PAHs in the nature is of great concern to human health as these contaminants are widely distributed in the environment and are known to be toxic, mutagenic and carcinogenic. In the past decades, various passive sampler devices (PSDs) have been developed to concentrate hydrophobic organic compounds (HOCs) from environmental matrixes and to mimic bioconcentration. Previous research has indicated that triolein embedded cellulose acetate membrane (TECAM) and petroselinic acid embedded cellulose acetate membrane (PECAM), types of lipid containing membranes as well as samplers made of polydimethylsiloxane (PDMS) have potential to accumulate certain polycyclic aromatic hydrocarbons (PAHs) from water and soil and to estimate the bioavailability of these pollutants to living organisms. The present study compares the ability of this suite of passive samplers to mimic uptake of 15 PAH prioritised by the European Scientific Committee on Food (ESCF) by crop plants grown in a hydroponic nutrient solution.

MO 021

Use of the semipermeable membrane devices (SPMD) as integrative tool for monitoring polycyclic aromatic hydrocarbons in tropical seawater

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To understand the bioavailability of contaminants in any system it is necessary to measure the concentration of these contaminants. It can be done using an organism surrogate, or biomimetic model, such as a passive sampling device as semi-permeable membrane devices (SPMDs). SPMDs are membranes composed of low density polyethylene layflat tubing filled with a neutral lipid and have been shown to effectively mimic the function of lipid membranes in uptake of lipophilic contaminants. These devices have a number of advantages over live organisms including ease of deployment, low maintenance costs, transportability, and applications to a wide variety of environments.

In the two last decades, several works have been developed to measures polycyclic aromatic hydrocarbons (PAHs) in seawater by using this technique. However almost all of these studies were carried out in cold and oligotrophic waters from the North Hemisphere, where biofouling effect is minimized.

The purpose of the present study was to evaluate the use of SPMDs in tropical and eutrophic waters to measure PAHs as part of a bioaccumulation study near produced water discharges. This is particularly important due the necessity of monitoring seawater contaminats in the new offshore oil fields, including the Brazilian Pre-Salt.

Field studies to assess PAHs in the seawater by using SPMDs were carried out in the Potiguar basin, located at Rio Grande do Norte State, Brazil. The SPMDs were deployed in three different months of the year at five sampling points. Three sampling points were located near an ocean outfall which discharges produced water and two at 12 Km distant from the outfall, as a reference area. It was analyzed the EPA´s 16 priority pollutant PAHs and the respective homologue alkylated compounds. Near the outfall concentration of PAHs ranged from 25 ng L^{-1} to 623 ng L^{-1} with the presence of alkylated compounds from 2 to 4 rings and presenting PAHs distribution with weathering characteristics. At the control area the total PAHs concentration were quite similar to the SPMD blank, ranging from 0.8 ng L^{-1} to 4.8 ng L^{-1}.

PAHs concentration found in seawater near the outfall was within the concentration expected by the dilution model of the effluent. To sum up, based on this study, the SPMD technique has shown considerable promise in studies in tropical and eutrophic waters.

MO 022

Development and application of a passive sampling technique for determining biomagnification factors and elimination half-lives in fish following dietary exposure

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Recent revisions to the OECD 305 test protocol have led to the introduction of a dietary exposure test in which the bioaccumulation potential of a substance is characterized in terms of a lipid normalized biomagnification factor (BMF). The BMF expresses the lipid-normalized concentration ratio in fish tissue to that in the diet to which the fish is exposed at steady-state. Research was conducted to demonstrate the utility of passive sampling techniques for estimating BMFs and half-lives of several hydrophobic chemical in fish tissue following a dietary exposure in rainbow trout. In this study, five test substances (hexachlorobenzene, musk xylene, o-terphenyl, methoxychlor, benzo[a]pyrene) with a range of susceptibility to metabolic transformation by fish were selected to allow comparison of this approach to results obtained using conventional exhaustive extraction of diet and fish tissues. Method development consisted of determining optimal sampler volumes and equilibration times for chemical analysis of spiked diets, oils and fish tissue samples using disposable polydimethylsiloxane fibers (2 cm length by 100 µm film thickness) which were solvent desorbed and analyzed by GC-MS. Empirically derived lipid to PDMS partition coefficients ($K_{lipid\text{-}PDMS}$) were determined for fish feed, fish tissue, corn oil, and fish oil and found to be in good agreement across the four matrices for all compounds, with the exception of benzo[a]pyrene. These results were comparable to published research investigating $K_{lipid\text{-}PDMS}$ in lipids from various trophic levels. Laboratory derived BMFs and elimination half-lives determined using passive sampling techniques will be compared to results obtained using conventional

exhaustive extraction techniques. This approach offers a promising screening alternative test method for determining tissue concentrations, half-lives and biomagnification potential with potentially less fish and at a fraction of the cost than traditional test protocols.

MO 023
Study of partitioning between lipid and passive sampling materials for equilibrium sampling
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Samplers consisting of two phases like semi permeable membrane devices (SPMDs) as well as single phase polymer samplers (e.g. polydimethylsiloxane (PDMS), low density polyethylene (LDPE)) are widely used for monitoring of hydrophobic contaminants in the aqueous environment. Application of such passive samplers can be extended to monitoring of hydrophobic contaminants in fish tissue. Equilibrium concentration in PDMS sheets immersed in fish tissue can be easily converted to a concentration on lipid basis using separately determined lipid-PDMS partition coefficients. Such concentration in lipid showed a good relation with lipid-normalized concentration measured with classical analysis. So far, limited data on partition coefficients between lipid and passive sampler (Klps) are reported in literature. Klps can be calculated as the ratio of contaminant concentration in each phase at equilibrium. In the present work partitioning of major groups of hydrophobic contaminants as PCBs, PAHs, BDEs and various pesticides between several polymer materials (e. g. PDMS, LDPE) and various lipids (e. g. olive, fish, seal oil and a model lipid, triolein) is studied. The influence of temperature on the Klps is investigated. Equilibrium is confirmed by using performance reference compounds (PRCs) with properties equal to the properties of target compounds. Target compounds and PRCs are dosed to different media and an equal distribution of both compounds after equilibration demonstrates that equilibrium is achieved. Additionally diffusion of lipids in passive sampling materials at different temperatures is measured, including characterization by analysing the lipid patterns. The Klps values will contribute to implementation of monitoring in biota through passive sampling. Additionally when combined with existing water-LDPE partition coefficients, the obtained triolein-LDPE partition coefficients also allow to estimate water-SPMD partition coefficients for comparison with values presently applied in water passive sampling.

MO 024
Implementing WFD biota standards - a possible role for passive samplers?
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Environmental Quality Standards (EQS) define tolerable upper limits for concentrations of chemicals in the environment. For some substances, there is now the option of monitoring compliance in the body tissues of aquatic biota, or sediments. This may offer a more reliable and cost-effective measure of potential environmental risk than measurements in the water column for substances that bio-accumulate strongly and have very low aqueous EQSs.
Under the EU EQS Daughter Directive (EQSD), biota standards have been set for:
- mercury;
- hexachlorobenzene (HCB); and
- hexachlorobutadiene (HCBD).
The EQSD also sets out a requirement to monitor temporal trends of the levels of substances in biota and/or sediment.
The use of biota for assessing compliance and trends presents a number of challenges, e.g. choice of appropriate species, availability of species at different sites, and the destruction of large numbers of fish or invertebrates to collect the required data. We are not yet at a stage where we can implement biota standards with confidence.
To address these concerns, we are exploring alternative ways for assessing compliance with biota EQSs. Passive Sampling Devices (PSDs) are an emerging technique that could provide useful data on compounds present in the water environment without the requirement of sacrificing fish. To develop more confidence in a strategy for implementing biota standards and trend monitoring under the WFD, we need to compare the uptake of compounds in sediment, water, PSDs and biota (fish and mussels) sampled at the same sites at the same time.
Our poster describes a study to determine the potential role of PSDs as surrogates for biota. If quantifiable relationships can be discerned between chemical residues in biota, sediment and PSDs, we may be able to use PSDs as a surrogate for biota when assessing compliance with biota EQSs.
PSDs and caged fish (Leuciscus idus) or mussels (Mytilus edulis) have been deployed at a number of sites along the River Thames (freshwater and estuarine) and water and sediment samples have also been taken from the same locations. Analyses were conducted to determine the concentration of 13 compounds, including, HCB, HCBD, Pentachlorobenzene and TBT in all four matrices. The results from the trial and the potential for using PSDs for assessing compliance with biota standards and for trend analysis under the WFD will be presented.

MO 025
Measuring contaminant partitioning in Norwegian rivers
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Chemical monitoring under legislative structures such as the European Water Framework Directive (WFD) heavily relies on the application of environmental quality standards (EQS). Under the WFD, EQS values for hydrophobic organic priority substances have been set for the "whole water". Conventional sampling-analytical methodologies fail to meet target performance criteria for WFD method selection. Passive sampling devices are able to provide improved limits of detection (when compared with bottle sampling) and time-integrated measurements. However, concentrations measured with passive samplers are for the truly dissolved fraction and do not include those bound to particle or dissolved organic matter (i.e. the "whole water"). Reconciliation between passive sampling measurement and EQS is needed. Derivation of EQS values for the truly dissolved phase is a long-term option. A shorter-term initiative may be to estimate river-specific suspended particle matter-water partitioning coefficients. These may be based on measurements in the dissolved phase with passive samplers combined with techniques such as continuous flow centrifugation and in situ integrative SPM samplers. In this study, we have measured with the help of semipermeable membrane devices, silicone strips and low density polyethylene membranes dissolved phase concentrations of a range of nonpolar priority substances in 6 river of the South East of Norway. These measurements were complemented by measurements in the suspended particulate fraction. Contaminant partitioning coefficients were estimated from these measurements and put in context with literature data. Variability in partition coefficients were estimated with repeated seasonal sampling in 2 of the rivers over a 2 year period. We propose here to derive estimates of whole water concentrations based on passive sampling measurements. Uncertainties associated with for example contaminants sorbed to dissolved organic carbon are discussed.

MO 026
Development of passive surrogate addition devices for remote water sampling
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Most procedures for sampling remote bodies of water require the collection and shipment of the water samples from the site to the laboratory. In addition to the cost and inconvenience of collecting, bottling, preserving and shipping the water, there are possibilities for cross-contamination and errors at each step in the process. In another scenario, analytical instrumentation is available that is designed to be deployed in the field so that the analyses occur at-site. This second scenario for field testing is of course limited to the types of techniques supported by the instrumentation. A third scenario is the extraction of analytes from the water followed by shipment of sample-loaded concentration devices to a remote lab for analytical testing. We are most interested in this third scenario due to the potentially lower cost and complexity and we report on our efforts to improve and perhaps validate data quality for this type of system by developing a passive surrogate addition device.
A surrogate is a compound or analyte that is added to all samples during preparation. The use of a surrogate is required in most sampling procedures that are approved for environmental testing in order to insure that the method is actually delivering data in the 70-130% recovery range. A surrogate generally has similar properties and responses in the analytical process to the target analytes and can be used to prove that the process is both capable and actually did deliver quality data.
In remote sampling, there can be an issue with providing sufficient energy to power instrumentation including sampling pumps, valves etc. This can be easily solved by supplying a dual solar/battery power supply combined with consumption-minimizing components. If the system contains a mechanism for the addition of one or more method surrogates then one option is the use of a metering pump which of course would require power. In this poster we discuss our development of several passive systems for the addition of organic surrogates to sampling streams.

MO 027
Ambient thermal desorption ionization for rapid mass spectrometric analysis of contaminants
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To ensure the safety of consumers following an oil spill, a rapid screening method is required to analyze food for compounds of concern. Of the many compounds found in oil, a subset of major concern is the polyaromatic hydrocarbons (PAHs). These compounds are known to be carcinogenic and the US Environmental Protection Agency has defined these compounds as priority pollutants.
The application of ambient desorption techniques for sample introduction into mass spectrometers is an emerging technology that has applicability in many areas of contaminants analysis. The atmospheric-pressure solids analysis probe (ASAP) is a unique mass spectrometry technique for direct analysis of volatile, semi-volatile, solid and liquid samples. In ASAP, samples are introduced to the mass spectrometer on a glass capillary and vaporized with heated nitrogen desolvation gas. Ionization is achieved using a corona discharge. While conventional analytical tools, such as LC or LC/MS, require time-consuming sample preparation procedures, ASAP can provide mass spectra within seconds of sampling.
The use of ASAP coupled to a tandem quadrupole mass spectrometer for the detection of PAHs in seafood samples was investigated. Spiked samples of fish and shrimp were homogenized and then sampled directly with the glass capillary. PAHs were screened using multiple reaction monitoring (MRM) mode. In addition, PAHs were extracted from

the samples using a simple QuEChERS protocol and the extract sampled directly using the capillary. Results from both approaches will be presented. This work provides an interesting example of the potential applications of ASAP for the analysis of environmental contaminants and will discuss the benefits and challenges of the technique.

MO 028

Development of a communicating portable analytical system of organic micropollutants in water based on UV spectrometry-fluorimetry detection after multiple solid phases selective preconcentration

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Lots of organic contaminants such as regulated molecules (phytosanitary products, polycyclic aromatic hydrocarbon (*PAH*), [3DOTS]) as well as emerging pollutants (pharmaceutical products, endocrine disruptors, [3DOTS]) are generally present at trace level in environmental waters (in particular natural waters) except in case of accidental or intentional pollution where concentrations are stronger. In general, detection methods include, sampling, solid phase extraction (*SPE*) and finally gas or liquid chromatography-mass spectrometry (*GC-MS* or *LC-MS*) (Hilton *et al.* 2003, Momplaisir *et al.* 2010). These protocols are necessary because standardized, but, they are limited when sudden pollution/contamination occurs and when rapid decision making is required. In this case, there is a growing interest to have available, rapid and on site detection techniques able to give information (qualitative, (semi)quantitative) of the type of pollution and the potential corresponding hazard for the environment and human health.
In this work, we develop a rapid, reliable and low cost solution for the detection of organic micropollutants directly on site, based on multiple solid phases selective preconcentration (*MSP2*) coupled to UV/Visible spectrometry and/or fluorimetry.
The principle of the development is to combine several solid phase preconcentration cartridges (different chemical sorbents can be used) and various washing/elution solvents for the on site extraction, separation and detection of specific chemical micropollutants or family of substances.
A first approach have considered 13 substances among which pesticides, pharmaceutical products, *PAH* and endocrine disruptors in more or less complex mixtures. From the physico-chemical (pk_a, K_{ow}) and optical (UV and fluorimetric spectra) proprieties of each target, and by mixing several sorbents and elution solvents, we tried to propose protocols for the detection of each component in the considered mixtures.
Such system can be characterised by its availability (rapid use and result in real time), simplicity (easy to transport and use by everybody), and rapidity (adapted procedure based on simple principle).
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MO 029

Ultra low level determination of bisphenol A, 17-β estradiol and poly aromatic hydrocarbons in river water using fully automated column-stitching HPLC

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Automated solid phase extraction (SPE) is one of potential candidates for improving experimental productivity. We have reported novel auto-SPE column-switching HPLC method for the determination of trace amounts of chemical substances in surface water using specific detectors such as mass-spectrometry (MS), along with electrochemical detector. Bisphenol A (BPA), which has been suspected as an endocrine disruptor and 17-β estradiol, (E2) most famous natural estrogenic compound were determined at ng/L levels with this method[1, 2]. Here we have introduced multi-valve column switching HPLC system with a specially designed pretreatment column[3]. This column-switching system solved a recurrent issue of column clogging and the pretreatment column provided remarkable performance for removal of humic compounds from environmental water samples. Use of this combination controlled ion suppression and increased peak response while using single stage MS as a detection system.
On the other hand, there is still a demand to do trace analysis with simple and inexpensive way. We found it possible to detect ng/L levels of BPA and poly aromatic hydrocarbons (PAHs), which are described in EPA method 610 with fluorescence detector. PAHs show strong hydrophobic nature and they can be often adsorbed on the surface of HPLC flow line especially resin-made parts. To avoid this phenomenon during auto-concentration, we employed "dilution-concentration"device, which provided reliable recovery and repeatability. Typical performance parameters of this system with fluorescence detector were validated.
Real water samples were collected then BPA, E2 and the PAHs were determined at ng/L levels with excellent repeatability and sensitivity by using proper detection way respectively. Hence, such switching techniques can be used for trace level analysis of environmental contaminants, carcinogens and additives in varied samples with complex matrices. These techniques may therefore assist in sample clean-up, target compound concentration, separation etc. An appropriate choice of a sensitive detection system can afford to carry out ng/L and sub-ng/L levels analysis with ease and required sensitivity.
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MO 030

HPLC analysis of isocyanate aerosol in workplace

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Workplace atmosphere is an important distribution of various pollutants, resulting from the handled products and concerned processes. The fate of these pollutants in the air (transport, deposition, degradation), is determined by their distribution between atmospheric particles and gas phase (Lohmann et al. 1998). Harmfulness of particles in workplace atmosphere and the disease hazards that they present are related to their chemical nature and size. The production of one kilogramme rigid polyurethane foam releases nearly 7362 milligrams of solid particles in air.
In this work, we used the personal aerosol sampler CIP10-R (Courbon et al. 1988) and filters for evaluation of alveolar (Gorner et al. 1996) and inhalable fractions of particles during clean of casts after injection of the polyurethane foam (PU). HPLC was used for detection of MDI in different post.
Obtained Results reveal that MDI in alveolar fraction prevail the total collected particles, this can be allotted to the process used for cleaning and to the quality of formulated foam.
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MO 031

Development and calibration of a passive sampler for N-nitrosodimethylamine (NDMA) in water

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N-Nitrosamines such as N-nitrosodimethylamine (NDMA) are organic compounds of contemporary interest in environmental waters, including groundwater, wastewater and potable water, due to their potent carcinogenicity in laboratory animal studies and probable human carcinogenicity. Heightened awareness of their properties and prevalence has led to increased scrutiny of water with Maximum Contaminant Level (MCL) goals ranging from 2 ng L-1 in California to 9 and 10 ng L-1 respectively in Canada and Australia and quantification limits down to low ng L-1 levels.
USEPA Method 521 [1] for the analysis of N-nitrosamines in water is a coconut charcoal-based solid phase extraction method. This work investigated the use of the charcoal specified in this method as a passive sampler sorbent for NDMA and stipulates its use for other nitrosamines.
The suitability of coconut charcoal as a sorbent phase for NDMA has been previously investigated. However, this involved simple batch experiments. To employ it in a passive sampler, calibration data such as sampling rates (RS L.day-1) and sampler-water sorption coefficients (KSW) applicable to environmental conditions must be available for target compounds. In addition, these calibration characteristics should be independent of ambient concentrations. The aim of this study then was to develop and calibrate a passive sampler for NDMA using coconut charcoal as a sorbent phase.

MO 032

'Wa-shi' (Japanese paper) fabrics as adsorbents

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A traditional Japanese paper, "Wa-shi"has been strained from bark of some tree or shrub. The ward "Wa"means Japanese, whle "shi"means paper to describe paper made by hand in the Japnese traditional manner. Wa-shi is mainly utilized in traditional arts, such as Origami or Shodo.
Recently fabrics were made using Wa-shi. Some special method realized various types of Wa-shi fabrics and commercialized by a Japanese company, CURETEX [1]. One of the recent tpics of Wa-shi fabrics was socks, which were utilized in space by a Japanese female astronaut to proof moisture retention as well as deodorization.
The detailed mechanism for above characteristics has not been elucidated yet, but Wa-shi is simply made from cellulose, therefore, adsorption abilith is probably possessed. In addition, textile forms and/or knitting things are really suitable for fast adsorption of environmental water. In this paper, we wish to show fundamental adsorption ability of the fabrics of Wa-shi (Japanese paper) as envionmental clean-up device. As the result rather fast adsorption for a dye was observed inspite of loose textures.

MO 033

Mass balances and passive dosing of polychlorinated dibenzo-p-dioxins in a cell based bioassay
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Persistent organic pollutants are ubiquitous environmental contaminants and pose health risks. Cell-based bioassays could be cost-efficient and ethical alternatives to animal testing in chemical risk assessment. However, hydrophobic organic chemicals may appear less potent than they really are because their biovailability is reduced by sorption to growth medium and vials. In the present study we use the CAFLUX assay, which is specific for chemicals binding to the aryl hydrocarbon receptor and detects chemicals with a dioxin-like activity. For a series of polychlorinated dibenzo-p-dioxins we have assessed bioavailability and partitioning between medium components and cells and demonstrate how the partitioning affects the cellular concentrations with more than 99% of the chemicals sorbed to medium components thus reducing the sensitivity of the assay. We also demonstrate how to overcome this limitation with a novel dosing technique where the polychlorinated dibenzo-p-dioxins are desorbed from a polymer.

MO 034
Passive dosing as a tool to recreate the environmental mixture composition of HOCs in an aquatic toxicity test
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The general aim of this study was to explore the potential of passive dosing for testing the toxicity of a PAH mixture that recreates the mixture composition found in seawater from a coastal area of Spain, the Bay of Algeciras. First, solvent spiking and passive dosing were compared for their suitability to determine the acute toxicity to *A. franciscana* nauplii of several PAHs at their respective solubility limits. Second, passive dosing was applied to recreate the seawater mixture composition of PAHs from a Spanish monitoring program, and to test the toxicity of this mixture at different levels. HPLC analysis was used to confirm the reproducibility of the dissolved exposures concentrations for the individual PAHs and mixtures. This study shows that passive dosing has some important benefits in comparison with solvent spiking for testing hydrophobic organic compounds (HOCs) in aquatic media. These include maintaining constant exposure concentrations, therefore higher reproducibility and a relative increase in toxicity. Passive dosing is also able to faithfully reproduce real mixtures of HOCs, such as PAHs, in toxicity tests, reproducing both the levels and proportions of the different compounds. This provides a useful approach for studying the toxicity of environmental mixtures of HOCs, with a view to investigating their toxicity but also for determining safety factors before such mixtures result in detrimental effects.

MO 035
Speciation of PAHs in stormwater
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Partitioning to particulate matter and dissolved organic carbon (DOC) has a large influence on the transport and fate of hydrophobic organic chemicals in aquatic environments. In this study a newly developed method for studying speciation of hydrophobic organic compounds, called passive dosing, was used to measure partitioning of fluoranthene in samples of stormwater runoff. The freely dissolved concentration of 14C-fluoranthene in the samples was controlled by passive dosing from a pre-loaded polymer phase and the total sample concentration at equilibrium was measured. This method reveals the free fraction of fluoranthene in the sample as well as the enhanced capacity of the sample to carry fluoranthene relative to pure water. Free fractions of fluoranthene in the stormwater samples varied from below 15 % in the first sample from each event to 20-50 % during the last part of the events. Enhanced capacities of the stormwater samples for fluoranthene transport ranged from 2-23 relative to pure water. In the stormwater samples partitioning to the organic part of the suspended solids, measured by loss on ignition (LOI), dominated partitioning compared to partitioning to DOC. Even though samples were taken at different events and at different times during the events, partitioning to LOI remained constant with KLOI = 154000 ± 3000 L/kg. These results can be used in stormwater quality modeling and assessment of the efficiency of stormwater treatment systems.

MO 036
Application of passive samplers for monitoring of cyanotoxins in drinking water
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Massive proliferations of toxic cyanobacteria in drinking water reservoirs represent a serious human health hazard requiring effective tools for assessment and management of health risks resulting from eventual contamination of drinking water with cyanotoxins. Passive sampling is very perspective approach which could be effectively utilized for purposes of environmental and regulatory monitoring of cyanotoxins. Although passive samplers had been succesfully developed and/or evaluated for the most prominent cyanotoxins including microcystins, so far they have been only rarely used in research and monitoring of cyanotoxins.
This study is an example of our recent attempt to further extend the application of passive sampling techniques in the field of cyanotoxin research and regulation and especially to introduce this approach to drinking water treatment industry for control and management of cyanotoxins. In this study, we employed passive sampling alongside traditional techniques to monitor cyanobacteria and microcystins in two different drinking water reservoirs and adjacent drinking water treatment plants in the Czech Republic. During the sampling period Jul-Nov 2011, passive samplers were biweekly deployed/replaced and grab samples collected from open reservoirs and from different stages of water treatment process (raw water, flocculation, clarification, filtration, final treated water). Phytoplankton species composition and quantities were determined microscopically as well as by submersible fluorimeters. Microcystin concentrations were determined in both grab samples and exposed passive samplers by HPLC-DAD and/or immunochemically (ELISA). The poster will compare data obtained from both sampling approaches (passive/grab sampling) as well as discuss and demonstrate potential and limitations of passive sampling techniques for monitoring of cyanotoxins in drinking water, drinking water quality control, evaluation of efficiency of cyanotoxin removal during particular steps of the drinking water treatment process, and human health risk assessment. This study should facilitate future applications of passive sampling techniques in water quality monitoring practices.
The research was supported by the SoMoPro project no. 2SGA2858 (funded from the European Community within the Seventh Framework Programme (FP/2007-2013) under Grant Agreement No. 229603 and co-financed by the South Moravian Region).

MO 037
Field evaluation of chemical probes to determine the fate of persistent organic pollutants in soil
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Persistent organic pollutants (POP) such as polycyclic aromatic hydrocarbons (PAH) and polychlorinated biphenyls (PCB) usually enter the atmosphere either in their gaseous form or sorbed to carbonaceous and/or other organic matter containing particles. Long-range atmospheric transport and deposition (wet and dry) lead to a ubiquitous distribution of POP in the environment. POP accumulation in low temperature environments such as the polar regions and mountains is described as cold trapping. In addition, a fractionation of volatile compound mixtures can be seen toward the poles which is probably due to climate-controlled desorption, evaporation and re-deposition processes ("hopping"). It was hypothesized that especially at high altitudes of mountains remobilized contaminants may accumulate and contaminant patterns may change, in order of the contaminants physico-chemical properties. In our study we used PAH and PCB as model compounds to study climate and altitude triggered fractionation processes in detail under field conditions. In a remote alpine valley in the European Alps and in a valley in the Black Forest Mountains (Germany) test sites at various altitudes were equipped with chemical probes. These consisted of a porous ceramic tube (pore size ca. 5 nm) which were filled with various materials (quartz sand, peat and charcoal) to mimic different desorption scenarios from sorbents with varying sorption capacity. The materials were spiked with defined contents of PAH and PCB (20 mg/kg and 1 mg/kg) and the chemical probes were buried in soil in a maximum depth of 5 cm below surface. After several months the tubes were analyzed for evaporative PAH and PCB losses. After a total study period of 1 year, we found for quartz sand losses of volatile compounds such as naphthalene or phenanthrene close to 100% within the first 9 months at all altitudes. Fluoranthene showed a slight decrease of loss with increasing altitude which is in line with a expected fractionation. For stronger sorbents, e.g. charcoal and peat, losses were much smaller and for some tubes even an increase of the loading was observed. Higher-ring-PAH showed no loss or the results were within the analytical error. The PCB with high volatility showed 100 % loss after a 9 month period of deployment, while PCB with lower volatility showed a decreasing loss with increasing altitude. This result could be confirmed from chemical probes analyzed after 12 month of deployment.

MO 038
Seasonal and temporal trends of airborne POPs around a waste incineration plant by passive sampling methods
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High-volume active samplers have been conventionally used for the environmental monitoring of persistent organic pollutants (POPs) in air. However, these systems have several drawbacks, such as high cost or power need. Consequently, alternative methods, such as passive samplers, are being developed, as semi-quantitative measures complementing active systems. Due to the low cost and easy handling, polyurethane foam (PUF) disks are especially attractive. PUFs seem to be a useful tool to compare the state of pollution in specific areas, as well as for seasonal and spatial distributions of local POPs. In 2010, an environmental monitoring program of the municipal waste incinerator (MSWI) in Tarragona (Catalonia, Spain) was initiated by measuring the immission levels of polychlorinated dibenzo-p-dioxins and dibenzofurans (PCDD/Fs), polychlorinated biphenyls (PCBs) and polychlorinated naphthalenes (PCNs) by means using passive samplers. In order to establish seasonal and temporal trends, four campaigns (between March 2010 and September 2011) were carried out. PUFs were deployed for 3 months at 8 different locations around the facility. Levels of PCDD/Fs ranged from 0.007 to 0.038 pg WHO-TEQ/m3, being very similar to those previously reported in the scientific literature. Regarding PCBs, the concentration of dioxin-like congeners was comprehended between 1.38 and 3.75 fg WHO-TEQ/m3, and the average levels of the 7 environmental marker PCBs was 44.1, 38.9 and 30.2 pg/m3 along the three first studied campaigns. PCN levels presented very similar levels through the program, with values ranging 6.45-6.95 pg/m3. While no temporal and seasonal patterns were noted in the airborne concentrations of POPs, the current levels of PCDD/Fs, PCBs, PCNs in air near MSWI are below or similar to those reported in other references sites, and typical of semi-urban areas.

MO 039
Can car cabin air filters be a useful a sampling medium for air pollution monitoring purposes?
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This study presents for the first time results of gas-chromatographic chemical analysis of car cabin air filters (CCAFs) collected from typical UK cabs from the city of Manchester, United Kingdom. As a first step, this study focuses on polycyclic aromatic hydrocarbons (PAHs), the most important category of semi volatile organic pollutants associated with traffic emissions.
Concentrations of ΣPAHs in CCAFs ranged between 2760 and 10800 μg/filter, with benzo[b]fluoranthene, benzo[k]fluoranthene and indeno[123-cd]pyrene being the most abundant PAHs. Benzo[a]pyrene (BaP) ranged between 315 and 740 μg/filter, accounting regularly for 5-15% of the total PAHs. Atmospheric BaP (and other PAHs) concentrations were estimated by using different scenarios for ventilation rates, and duration of filter's exposure and it was shown that the BaP levels of the air that CCAFs collect can exceed the guideline value of 1 ng/m3 up to 100 times.
Calculation of PAHs molecular diagnostic ratios shows the predominance of traffic related emissions.
We conclude that CCAFs are an invaluable alternative to conventional air sampling methods, featuring unique advantages, that are a) the exposure estimation of car passengers, riders, pedestrian or road-professionals, b) unlimited sample size, ideal for screening of the air quality, especially for compounds that tend to partition on particles, c) provide with an average, time weighted urban air pollution assessment. The main disadvantage of this method is the uncertainty associated with accurate estimations of atmospheric pollutants concentrations, due to lack of knowledge of the exact amount of air filtered, and the fact that vehicles are used also for trips to less polluted places and/or the fact that also the recirculation of car cabin indoor air is undergoing filtration.

MO 040
Observations on flame retardants (FRs) in indoor environments in Istanbul-Turkey
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Due to the several indoor sources of flame retardants-such as upholstery textiles and foam paddings in furniture and matresses, thermoplastics for computers, TVs, electrical components and cables-indoor air is a very important exposure route of flame retardants (FRs). As they are less subject to photoloysis and atmospheric dilution in indoor environments, they show increased air concentrations. Like outdoors, data of POPs indoors are sparse or lacking in Turkey. In this study we investigate PBDEs and non-PBDE novel flame retardants in houses, offices, electronics shops and upholstery+matress shops indoor air and dust samples. The air samples were collected by using indoor air passive samplers. Dust samples were collected by vacuuming a 2 m2 area for 4 minutes. The main objectives of this study were a) utilization of polyurethane foam disc (PUF) passive sampling technique for indoor environments, b) to start the database on concentrations of flame retardants in indoor air and dust in Turkey, c) to investigate the congener profiles and partitioning of flame retardants in indoor environments, d) to evaulate flame retardants exposure through indoor air and dust pathway. For these purposes, the planned study is in progress and samples analysis is being carried out at the present.

MO 041
Comparison of four modeling approaches to describe chemical uptake by passive air samplers
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Over the past decades, various passive air samplers (PASs) have been developed to monitor semivolatile organic compounds (SVOCs) in air. Uptake in PAS occurs by molecular diffusion from air to a passive sampling medium (PSM), such as polyethylene (PE), polymer-coated glass (POG), polyurethane foam (PUF), and XAD-resin. Unlike in PE or POG-based PAS, where SVOCs accumulate in thin layers in contact with air, PUF and XAD are porous materials. The Whitman two-film model, which was originally developed to describe mass tranfer between air and water, is often used to decribe chemical tranfer from air to the PSM. This model requires that "*in the main body of either liquid or gas [[3DOTS]] the concentration of solute in the fluid is essentially uniform at all points.*"While this assumption may be satisfied when modeling chemical uptake by thin, non-porous PSM such as PE and POG, it is unlikely to be valid for thick, porous PSM such as PUF and XAD. Chemical transfer within such PSM only occurs in the gas filled pores, which limits the transfer kinetics because only a low fraction of the SVOCs is in the gas phase. Recent experimental evidence confirms that SVOCs do not distribute uniformly within the PUF and XAD, which therefore directly contradicts the assumption of the two-film model used to describe chemical uptake by PUF- and XAD-PAS. The two-film modeling approach for PAS is also not able to explain the sampling rate decrease that has been observed during the initial uptake phase of a few calibration studies involving PUF-PAS. In this study, in order to seek an alternative approach to modeling chemical uptake by PUF- and XAD-PAS, we compare the two-film model with three other approaches that are commonly used to describe intermedia mass transfer of chemicals. These approaches either (1) describe uptake within the PSM using an effective diffusivity of chemical transfer within porous media assuming an average diffusion length within the PSM, or (2) assume the existence of two types of binding sites within the PSM which contribute to fast and slow uptake, or (3) are based on Fick's diffusion law for chemical tranfer in air and in porous media.

MO 042
Layer by layer self-assemble acetylcholinesterase and gold nanoparticles on glassy carbon electrode for sensing organophosphate pesticides
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Organophosphates(OPs) are highly toxic compounds to the vertebrates, which can be absorbed readily through the skin, mucous membranes, gastrointestinal and respiratory tracts. With the increasing awareness of environmental protection and health concerns, there is a growing public concern about the accumulation of OPs in food products and water supplies.
An sensitive amperometric biosensor for the determination of OPs based on Layer-by-layer (LBL) self-assembled acetylcholinesterase (AChE) and gold nanoparticles(AuNPs) on glassy carbon electrode(GCE) is described. The GCE is modified with AuNPs by electrostatic interaction between AuNPs and cationic poly(diallyldimethylammonium chloride) (PDDA). AChE is immobilized on the negatively charged AuNPs surface by alternatively assembling a PDDA layer and an AChE layer.
The unique sandwich-like structure (PDDA/AChE/PDDA) on the AuNPs surface formed by self-assembling provides a favorable microenvironment to keep the bioactivity of AChE. Owing to the inherent conductive properties of AuNPs, the immobilized AChE exhibited a higher affinity to its substrate and produced detectable and fast response. Electrochemical impedance spectroscopy of the AuNPs/PDDA/GCE and PDDA/{AChE/PDDA}2/AuNPs/PDDA/GCE indicate that AuNPs promote electron transfer and AChE is immobilized on the electrode surface successfully. The sensor performance, including inhibition time and pH, was optimized with respect to operating conditions. Under the optimal conditions, the inhibition rate (I %) of methyl parathion towards the immobilized AChE was proportional to the logarithm of the concentration over the range of 4.6[GREEKX] 10-5 to 5.3[GREEKX] 10-3 M with a detection limit of 7.6[GREEKX]10-6M. The biosensor has been applied for the determination of methyl parathion in spiked vegetable samples.

MO 043
Spatially resolved distribution of chemicals on equilibrium passive samplers for the elucidation of modes of sorption
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Equilibrium passive samplers are widely used in environmental monitoring programs as they are relatively easy to use and concentrations in air or water, respectively, can be easily calculated using the partitioning constants once chemical equilibrium is established (equilibration times depend on the dimension of the samplers, i.e. the thickness of the sampling media). This approach critically relies on the assumption that sorption on the sampling media is fully controlled by a partitioning process and, thus, the partitioning constant is independent from the concentrations (i.e. linear sorption isotherm). However, recent studies have shown that the partitioning constants on some equilibrium passive samplers (e.g., polyoxymethylene passive sampling devices) are higher when the thickness of the sampling media is reduced. Such observations are inconsistent with the partitioning theory, stimulating the idea that, apart from partitioning into the sampling media, additional interactions occur at the surface of the samplers (i.e., adsorption processes).
In this study, batch experiments were conducted with fluorene as probe compound and polyoxymethylene (POM) and polyethylene (PE) as sorbents. Subsequent to equilibration, the samplers were investigated using Raman spectromicroscopy in order to map the fluorene concentrations among the passive samplers. First results indicate that fluorene can be distinguished from the sampling media, which allowed mapping of the chemicals distribution on the surface of the samplers. Additional studies will focus on cross sections to investigate concentration gradients through the samplers to further elucidate the mode of sorption on equilibrium passive samplers.

EC04P - Novel approaches to addressing metal and metal nanomaterial bioavailability in soils

MO 044
Earthworm influence on metals bioavaibility in relation with metal speciation and ecotoxicity
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-Metal-enriched atmospheric fine and ultra-fine particulate matters (PM) are currently rejected in environment increasing significantly ecosystem pollution by metals. Few data are currently available concerning metals impact on environment and human health. In the context of Reach regulation, the study of pollutant fate and impact on the biosphere is required, as well as efficient tools development for sanitary risk assessment. Earthworm is a key organism to assess soil quality. By its bioturbation activities, earthworm could modify metal bioaccessibility and bioavailability in soils (in relation with metal localization and speciation). In this context, several experiments are performed to: (i) Estimate the difference of metals bioaccessibility and bioavaibility between polluted soils influence by bioturbation or not; (ii) Determine earthworm influence on metal speciation by studying ingested soils and casts; (iii) Asses ecotoxicology impact of metal from atmospheric PM on earthworms.

-Different PM and polluted soils (historically polluted and spiked soils); two species of earthworms: L. terrestris (ecologically relevant) and E. fetida (international standard for ecotoxicology tests) will be used for laboratory or field experiments. For the different soils before and after bioturbation: i) metal bioaccessibility will be determined by in vitro UBM test; ii) metal phytoavailability will be assessed by the study of plant uptake (lettuce); iii) microscopic (MEB-EDS) and spectrometric (Raman, XRF et Exafs) techniques will be used to perform elementary maps and determine potential changes in metal speciation (cast study); iv) general parameter like survival, biomass changes, cast production and burrowing activities will be studied to assess metal ecotoxicity.
-Strong influence of particle size and metal speciation on metal bioaccessibility was observed: variation between 20 and 82% according to experimental conditions. Moreover significant ecotoxicology effect on earthworm (using cast-production and biomass change measures) was highlighted.

MO 045
Investigations into the environmental bioavailability of lead in metal-rich granules produced by the earthworm Eisenia fetida
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Lead (Pb) is the most common metal contaminant found in the soils of small-arms ranges of US military instillations. Currently, risk assessors often assume that Pb is 100% bioavailable for ecological receptors, even though research has shown the modification of Pb bioavailability and toxicity by soil physicochemical characteristics and metabolism by organisms. Many terrestrial invertebrates are capable of rendering Pb toxicologically inactive through the formation of metal rich granules (MRGs). While Pb in MRGs is not considered bioavailable via trophic transfer, little is known regarding the fate of MRGs in the terrestrial environment once released from exposed organisms. The current research characterizes the microstructure of MRGs formed by the earthworm, Eisenia fetida and determines the potential for the microbial degradation and remobilization of Pb previously sequestered in MRGs. If liberated by bacterial degradation, sequestered Pb may become bioavailable to invertebrates and their predators. The direct bioavailability of Pb in MRGs to oligochaetes in soil will also be examined. Earthworms were exposed to soils spiked with 4,000 mg/kg Pb for a six-week period and fractionated utilizing differential centrifugation and digestion to separate whole-animal tissue from MRGs to obtain sufficient MRGs for amending soils for microbe and oligochaete exposures. Once extracted, MRG composition and concentration was analyzed utilizing synchrotron based analysis at Argonne National Laboratories (Argonne, IL). Synchrotron imaging provided multi-channel analyzer (MCA) plots which revealed localized MRG hotspots within the samples, not only confirming the presence of Pb, but also the binding of additional metals such as zinc and iron. Additionally, synchrotron techniques were utilized on cross-sections of earthworms to determine the presence and concentration of Pb across a gradient of dermal and gut tissue. MCA plots of cross sections revealed a wide dispersion of Pb inside the gut wall, suggesting the present of unbound Pb in addition to MRG formation. The results of the exposure of microbes and oligochaetes to Pb in MRGs will be discussed.

MO 046
Lead bioavailability to soil invertebrates as affected by soil physicochemical characteristics
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The bioavailability and toxicity of lead (Pb) to terrestrial invertebrates may be markedly modified by variations in the physicochemical properties of soil. Other factors that modify the toxicity of Pb include aging and leaching, yet most toxicity data are obtained from toxicity tests conducted with soils freshly amended with metal salts and the relevance of data from such tests to contaminated field soils is unclear. This study compares the chronic toxicity of Pb to Eisenia fetida and Folsomia candida in seven European soils varying widely in physicochemical properties (i.e., pH, organic matter content, texture, eCEC). Toxicity across all seven soils was compared using soils that were leached and pH corrected after freshly spiking with lead chloride. This was done to exclude the confounding factors of increased ionic strength and decreased pH due to spiking. Three of these soils (Barcelona, Ter Munck, Woburn) were also amended with lead nitrate in 2004 and aged under field conditions for five years prior to conducting laboratory toxicity tests and additionally tested directly after freshly spiking (without leaching or pH correction). These treatments allow for the estimation of leaching/aging factors to extrapolate toxicity from laboratory to field conditions. Highly significant correlations between log EC50 and log eCEC were observed for the E. fetida reproduction tests, but toxicity of Pb to F. candida was low and not affected by soil properties. Leaching and aging generally attenuated the toxicity of Pb to both soil invertebrates studied. The toxicity data, together with leaching and aging correction factors, provide important information on the bioavailability of lead to invertebrates in soil under realistic conditions.

MO 047
Lead bioavailability and bioaccessibility in sediments from wetlands with different hunting management in Tuscany (Italy)
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Lead (Pb) shot spent over wetlands causes Pb poisoning in waterfowl, which confuse it with grit for grinding function in the gizzard. Although often incorrectly regarded as inert, once dispersed in the environment, Pb shot undergoes a slow transformation into various molecular species that diffuse more readily in the environment and increase the bioavailability of the metal. Waterfowl species, which for their feeding habits probe into the sediment in search of food can steadily be exposed to Pb through the unintentional ingestion of contaminated sediment.
In this study we investigate the relative bioavailability and bioaccessibility of Pb in sediments from two Italian wetlands “Diaccia-Botrona”(costal wetland) and “Padule di Fucecchio”(inland marsh) where previous studies showed high Pb levels. Sediment was sampled from areas with different degree of Pb shot pellet densities in each wetland, including shooting ranges and hunting estates and natural reserves. The
relative Pb bioavailability was evaluated using the Community Bureau of Reference (BCR) sequential extraction procedure, whereas the relative avian Pb bioaccessibility was estimated by using an “in vitro”simulation of the gizzard-intestine system.
Pb partitioning obtained with BCR procedure showed a similar pattern for “Diaccia-Botrona”and “Padule di Fucecchio”. Percentage of total Pb concentration in sediment were less than 6% in the fraction 1 “acid extractable”with exchangeable and carbon bound metal, about 72-80% in the fraction 2 “reducible”with iron manganese oxide/hydroxide associated metal, about 4.25-16% in the fraction 3 “oxidisable”with metal bound to sulfide and organic matter, and about 3.5-18.6% in the fraction 4 “residual”with metal in the mineral phase.
Despite of the similar pattern of BCR partitioning of Pb in the two wetlands, results of “in vitro”simulation showed percentages of bioaccessible Pb in gizzard phase (pH 1.5) two order of magnitude higher for “Padule di Fucecchio”than for “Diaccia-Botrona”in both the shooting ranges (14% and 0.18%, respectively) and natural reserve areas (10.6% and 0.10%, respectively).
Due to the non-acidic conditions of the intestinal phase (pH 6.5), final Pb bioaccessibility were below of detection limits in both study areas.
According to these results, direct ingestion of Pb shot pellets can represent a higher risk for birds than the unintentional ingestion sediment contaminated by the disaggregated pellets in heavily hunter areas.

EM02P1 - Fate and exposure modelling

MO 049
Evaluation of a molecular fragment-based tool for predicting pp-LFER descriptors of complex and multifunctional organic compounds
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Poly-parameter linear free energy relationships (pp-LFERs) are useful models to accurately describe equilibrium partitioning processes of neutral organic chemicals in technical and natural systems. However, only a limited number of pp-LFER solute descriptors are available so far for complex and multifunctional compounds as well as for environmentally relevant substances. This hampers the application of pp-LFER models for estimating environmental partitioning behaviour of pollutants. The experimental determination of these descriptors is tedious and time consuming. Especially for screening purposes, the ability to predict solute descriptors just based on the molecular structure would be highly desirable.
The commercially available software ABSOLV is an easily accessible and manageable tool that predicts solute descriptors based on a SMILES input. Here we evaluate the performance of ABSOLV to predict partition coefficients using calibrated pp-LFER equations in combination with predicted ABSOLV descriptors. This evaluation is done for various partition processes and a large set of complex, multifunctional organic solutes.

MO 050
Model suite to estimate the air/water partition coefficient of organic compounds at 25°C
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The air/water partition coefficient K_{aw} is one of the key properties in environmental partitioning. A number of estimation models for K_{aw} are available from literature. However, despite of the number of recently published new experimental data, at least to our knowledge there was no relevant new model published within the last years. The poster first presents a critical review of the existing models through validation with a huge up-to-date data set. Furthermore, this set has been employed to develop three new models based on fragments, Abraham parameters, and read-across through atom-centred fragments.

The performance of the new models is presented, and the inter-correlation of the model errors for the different new and literature approaches is examined. Bundling all methods in a model suite thus allows for a sophisticated consensus modelling of K_{aw}.
All referred and new models are implemented and publicly available in the public free edition of ChemProp (see http://www.ufz.de/index.php?en=6738 for details).

The development of these models was partly supported from the EU Integrated Project OSIRIS (contract No. 037017).

MO 051
ChemProp - chemical properties estimation software system
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The software system ChemProp is an essential part of the outcome from the EU Integrated Project OSIRIS (contract No. 037017). It is publically available for free based on a bilateral license agreement (see http://www.ufz.de/index.php?en=6738 for details).
ChemProp comprises models to estimate compound properties and a database for chemical structures and properties, together with tools to manage compound sets. The QSAR part addresses models for physico-chemical properties with particular remark to partitioning processes of environmental relevance and degradation, environmental fate, ecotoxicological endpoints, and human toxicology. It mainly employs models based on the topological matrix and thus does not require quantum chemistry. Particular remark is given to the applicability domain, model uncertainty, and consensus modelling. The integrated database allows for structure and substructure searching, and addresses tautomerism and stereomerism. For effective data handling, it provides access to data in external resources in combination with the structure search facilities. It is linked to the public OSIRIS ITS webtool (http://osiris.simpple.com/OSIRIS-ITS/itstool.do).
The poster presents a general overview on ChemProp, and in particular emphasises new developments achieved since the poster presentation of ChemProp at the SETAC Europe meeting 2011 in Milan.

MO 052
ECETOC TRA: refinement of the OPS model parameters for the estimation of the chemical concentrations in environmental media due to atmospheric deposition
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The concentration of polluting substances in the air determines the intake through inhalation by humans. Deposition fluxes in soil, sediment and water determine environmental exposure which of course also indirectly affects humans.
In this poster, the exposure of water and air will be mainly focused due to deposition processes.
Dry and wet depositions from the atmosphere are estimated using the 2004 version of the ECETOC TRA (Targeted Risk Assessment) integrated tool based on the OPS model (Operational Priority Substances) model. The model is based on several assumptions to make it representative at a European level but does not necessarily systematically yield realistic exposure estimates.
A serie of different substances have been chosen differing by their different volatilities and it will be investigating the possibility and feasibility of refining various parameters of the model such as the source description, the emission height and the heat content of the emission plume, suggested by de Bruin et al. (2010). Deposition fluxes in the soil compartment will be calculated on the basis of these refined model parameters and discussed.

MO 053
Establishing a postgraduate course on exposure modeling for environmental risk assessment
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As part of the environmental risk assessments of chemicals, exposure assessments are required by various EU directives, e.g. those on plant protection products, on biocides, pharmaceuticals and on industrial chemicals. In the European community, the latter category is covered by the REACH legislation (Registration, Evaluation, Authorisation and Restriction of Chemicals), which prescribes industry to perform environmental exposure assessments for all chemicals on the market and report them in Chemical Safety Reports. Prerequisite to this is that expertise in enivironmental exposure assessment is available for regulators, industry and those who provide their service to industry. Environmental exposure assessments are performed in a tiered process. That means that assessments start simple and can be refined if necessary. First-tier assessment usually involves multimedia fate modeling to predict the concentrations of the chemical in the environment. Models use mathematical expressions to represent the emissions, the reactions and the transport processes that influence the chemicals' behavior in the environment. The basis of the mathematical representation for the tier-1 assessments in the EU is laid down in the REACH guidances R.10-R.16. Performing exposure assessments, as well as doing solid analyses of their results requires a complex set of skills. Basic understanding of the principles of exposure modeling is necessary to adequately interpret model results, such as predicted environmental concentrations (PECs). Understanding of the effects of input parameters on model output is essential. This more technical expertise needs to be brought together with the regulatory point of view. Therefore, individuals coping with regulatory aspects of environmental exposure assessment need to be trained in exposure modeling. We aim to establish a post-graduate teaching course that provides a thorough theoretical and practical insight in exposure assessment, using a set of acknowledged teaching materials. The goal of the designated postgraduate course is that participants gain (i) better understanding of scientific basis of exposure assessment under REACH; (ii) the ability to perform solid exposure assessments under REACH; and (iii) the competence to put exposure modeling into perspective. Course materials will be made publicly available.

MO 054
Parameter reliability in kinetic evaluation of environmental metabolism data - Assessment and the influence of model specification
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Currently, the usual way to determine parameter reliability in kinetic models fitted to environmental metabolism data includes a visual assessment, the determination of a relative measurement error level that may explain the residual variance based on a chi2-test and a t-test for significant difference of the parameter from zero. However, the kinetic rate constants can not be smaller than zero and therefore the assumption of a normal distribution is not appropriate. Furthermore, molar formation fractions can only take on values from 0 to 1. Therefore, also in this case a normal distribution can not be assumed. On this poster, several possibilities to overcome these problems are discussed.

MO 055
Development, application, and evaluation of models for screening organic chemical exposures to humans
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Chemicals are being evaluated to protect humans and the environment; however, there are few measured data available for the assessments. For the vast majority of chemicals, mass balance and Quantitative Structure-Activity (Property) Relationship (QSA(P)R) models are required to obtain data on chemical partitioning properties, persistence, bioaccumulation, toxicity (hazard), release rates, exposures to ecological receptors and humans, and risk. Uncertainty in chemical evaluations exists whether the data are measured or modelled and the uncertainty in the measured and predicted data for chemical screening assessments can be substantial. There is a need to address, quantify and ultimately reduce uncertainty in chemical assessments. The Risk Assessment IDentification And Ranking (RAIDAR) mass balance model was used to screen and rank a database of ~13,000 organic chemicals based on far-field human exposure. The model calculations included screening level uncertainty analyses to estimate the propagation of uncertainty in model input parameters on human exposure calculations. Three exposure metrics were selected here: the concentration in a human based on the actual emission rate estimate (CA), the concentration in a human based on an assumed, consistent unit emission rate for all chemicals (CU), and the intake fraction (iF). All of the endpoints are capable of discriminating several orders of magnitude differences in chemical exposure (CA) and exposure potential (iF, CU). In general, the exposure metrics (moving from iF, to CU, to CA) are shown to have increasing discriminatory power for screening purposes, increasing biological relevance for human exposure-based prioritization, but suffer from increasing uncertainty in their calculation due to reliance on additional model input data with high uncertainty (in particular, human metabolic biotransformation rates and emission rates). Efforts to reduce uncertainty in emissions estimates show reduced uncertainty in exposure estimates in revised screening simulations. The screening results from this holistic exposure assessment method are being evaluated with new and existing (bio)monitoring data and compared with screening results using persistence and bioaccumulation criteria. The approach provides a defensible method for identifying which chemical properties determine actual exposures and research needs to reduce uncertainty in the assessments. Research needs to improve the screening system are also highlighted.

MO 056
World exposure assessment tool
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A flexible modelling platform has been developed to evaluate the potential impact of crop protection chemicals on the environment throughout the world. The tool currently has been configured with scenarios containing crop, soil, and weather conditions for major agricultural areas in Canada, Colombia, the European Union, Norway, the People's Republic of China, and the United States. Scenarios are simulated using fate and transport models that have been accepted for regulatory assessment in the U.S. and the European Union, including the Pesticide Root Zone Model (versions 3.12.2 and winPRZM 4.51), EXAMS, RICEWQ, ADAM (groundwater dilution model), and TOXWA . A key strength of the tool is that scenarios can be added for additional geographical areas with relative ease and the appropriate regulatory endpoints.

MO 057
Uncertainty analysis using a Fugacity-based multimedia mass balance model: application of the updated EQC Model to D5
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Among several multimedia models, the Equilibrium Criterion (EQC) fugacity multimedia model has been widely used for the assessment of the fate, distribution and transport

of a chemical of interest in the environment. Since the model requires partitioning and reactive properties of the chemical as input data, it is very important to understand how much uncertainties of the physicochemical properties affect the model outcomes. Thus, this study focused on the uncertainty analysis of the EQC Level III model for decamethylcyclopentasiloxane (D5) to quantify the confident ranges of mass distribution, persistence and intermedia transport rates based on pre-determined dispersion factors of physicochemical properties of the chemical. For the uncertainty analysis, the Monte Carlo simulation technique was employed using Oracle Crystal Ball as an Excel Add-in program to a new spreadsheet platform of the EQC model.
The uncertainty analysis showed that once it is released or vaporized to air D5 stays in the compartment until it is removed at a relatively fast rate via OH radical oxidation and advection, resulting in relatively short overall persistence and no intermedia transport from air to other compartments. These model outcomes are not virtually affected by the uncertainties of physical properties of D5. On the contrary, when D5 is released to water, a major fraction is distributed in sediment due to sorption of the compound to organic substance in sediment where the degradation rate very small. In this case, the model outcome is predominantly influenced by the uncertainty of KOC.
Under a realistic emission scenario (94.5% to air, 0.8% to water and 4.7% to soil), the 95%-confident ranges of the mass distribution in air and sediment are 47%~78% and 19%~49%, respectively, whereas the overall persistence varies from 3.2 to 5.8 days with the same confidence. The variances are predominantly affected by KOC.
Overall, the EQC model results are strongly dependent on the mode of emission. Since the mass distribution in sediment is sensitive to the emission to water, accurate measurement of KOC and t½,Sed is expected to warrant a better understanding of the fate, distribution and transport of D5 in the environment.

MO 058
Multi-scale, multimedia modeling with Pangea - Local to global evaluation of the impacts of a distribution of coal power plants
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A large share of environmental impact and risk assessments of chemical emissions has been performed locally or regionally. However, it is usually not known how global impacts associated with these emissions do compare to local impacts. The present research focuses on the evolution of the intake fraction - the fraction of an emission that is ultimately taken in by the population - from local scale to global scale.
A review of existing models shows that currently published and operational models - ranging from single medium high resolution transport models to low resolution multimedia multi-pathway models - are neither able to properly reflect local to global impacts of emissions of pollutants, nor are they flexible enough to be adapted to specific locations or grid geometries. We already demonstrated innovative features of a new model called Pangea, aiming at adressing these needs, in a single-source context based on emissions of various types of plants located in the north-east of France. The present research provides a statistical result based on the study of more than 500 power plants located around the World, simultaneously demonstrating the flexibility of Pangea.
A set of multi-scale grids covering all the relevant media and refined around each source (coal power plants) are build. These grids allow Pangea to evaluate and compare local to global impacts of each source using a standard multimedia fate/transport and multi-pathway population exposure approach, but spatialized specifically for this study. Substances taken into account were chosen to represent broad categories of known environmental pollutants.
Results obtained so far for a few sources indicate that for volatile pollutants (e.g. Benzene) less than 10% of the overall population intake might happen within a 100km radius from the source, and hence that a local modeling (e.g. local risk assessment) of such emission might capture only a small fraction of the overall impact. We will present a statistical results on the comparison of local to global evolution of the integrated intake fraction. In other words, we will discuss statistically the fraction of the global intake that is captured by a local modeling, for a distribution of coal power plants (at their true locations) that covers the globe.

MO 059
Prediction of environmental and biological degradation half-lives with quantitative structure activity relationships
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Due to a general lack of measured information, predictive methods are required for degradation half-lives in environmental media and in biota to assist in chemical hazard and risk screening. Overall degradability of a chemical in the environment, calculated by the combination of chemical partitioning and environmental media-specific degradation half-lives, is a key determinant of chemical exposure and therefore potential risk. Depending on the partitioning properties, chemical usage, and mode of emission a chemical may be distributed differently in the environment which will alter its overall rate of degradation due to the differential rates of degradation in various physical compartments of the environment (i.e. air, water, soil and sediment). Chemical exposure potential to humans and ecological receptors is also dependent on food web structure, partitioning properties, route of exposure, and differential biotransformation rates of various biota comprising aquatic and terrestrial food webs. In order to interpret the overall role of chemical degradation on exposures, a multi-media multi-pathway mass balance model is required. Using RAIDAR, a multimedia mass balance exposure model linked with aquatic and terrestrial food webs, overall persistence and human and ecological exposures are evaluated as functions of chemical degradability in diverse environmental compartments and organisms. Quantitative structure-activity relationships (QSARs) are developed to cover as many different environmental media and biota as the current data availability allows. A novel algorithm to develop QSARs simultaneously for multiple environmental compartments and organisms is applied, and allows for a detailed analysis of the relationship between chemical structural features and exposure potential.

MO 060
Partitioning of organochlorines in storage lipids, membrane lipids and proteins in lean fish
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Lipids are the dominant force in determining organic contaminant accumulation in aquatic organisms because hydrophobic organic chemicals (HOCs) are believed to partition mainly into lipid phase. Therefore, lipid normalized tissue concentrations have been used to reduce variation in tissue residues between different species and aid in understanding of contaminant toxicity and distribution in food webs. However, partitioning of contaminants between different lipid classes is not very well known. Lipid composition contributes to variation in bioaccumulation potential and neutral storage lipids are thought to be the most important lipid class for HOCs. On the other hand, polar membrane lipids are the target for many HOCs toxicity and knowing the concentration in membrane lipids would greatly improve the risk assessment of HOCs. Using PDMS silicone as an partitioning phase, we have applied equilibrium partitioning approach to estimate HOC distribution in storage lipid, membrane lipid and protein fractions for carbon 14 labelled PCB-153, PCB-77 and PCP. The method is tested with the extracted native PCB contaminated pikeperch oil, and measures of lipid class and protein contents in fish. PCB distribution was dominated by storage lipids (70-78%) while membrane lipids (19-23%) and protein (2-6%) had lower share. The results showed the importance of chemical partitioning to protein fraction in lean fish. The results give new important insight of estimating toxicity by using chemical body burden as a dose metric.

MO 061
Simulating ionogenic chemical fate, bioaccumulation and exposure with RAIDAR
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Globally, chemicals are being evaluated for potential hazards and risks to ecological receptors and humans. When measured data are not available, multimedia mass balance models and Quantitative Structure-Activity Relationships (QSARs) are needed to estimate chemical concentrations in the environment and organisms. Fugacity-based multimedia models have been used extensively for simulating the environmental fate and bioaccumulation of neutral organics; however, exposure models are limited for ionogenic organics. It is estimated that approximately 50% of the 149,000 substances submitted under REACH are ionogenic. The lack of integrated tools for the evaluation of data-poor, ionogenic substances for the complete exposure pathway (i.e. emissions, to fate and transport, to bioaccumulation in aquatic & terrestrial food chains) reduces confidence in chemical assessments for substances that are subject to ionization in the environment such as many personal care products and pharmaceuticals. The Risk Assessment, IDentification And Ranking (RAIDAR) model includes linked fugacity-based multimedia fate and bioaccumulation sub-models, thus providing the capacity to evaluate exposures to humans and ecological receptors in a "holistic"manner. The general objective of this project is to revise and evaluate the RAIDAR model for the simulation of ionogenic chemicals for screening-level assessments. A secondary objective is to develop strategies to address chemical property data gaps so that the model may still be used under data-poor conditions. This presentation outlines the model revisions and explores the fate, bioaccumulation and exposure potential of ionogenic chemicals released to the environment. A hypothetical set of ionogenic chemicals are used to simulate how changes in chemical partitioning properties and dissociation constants affect chemical distribution in the environment and thus exposure potential to selected ecological receptors of interest (i.e. fish, piscivorous bird). Simulations are also conducted for current ionogenic chemicals of interest. These simulations highlight data needs for future research to improve model predictions to reduce uncertainty in the assessment of ionogenic chemicals.

MO 062
Predicting the oral uptake efficiency of chemicals in mammals: extension to the hydrophilic range
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Environmental risk assessment requires models to estimate bioaccumulation of untested compounds. So far, most mechanistic bioaccumulation models have focused on very lipophilic compounds, and only few included also more hydrophilic compounds. As shown by pharmaceutical studies, the membrane permeation of polar compounds is not sufficiently reflected by the octanol water partition coefficient (KOW). Therefore, additional descriptors are needed to mechanistically estimate membrane permeation.
Our aim was to develop a model to estimate oral uptake efficiency of pollutants via ingestion in mammals for polar and nonpolar compounds over a wide KOW range of pollutants with focus on polar compounds. The model was based on mechanistic processes and thus included the advective transport of the pollutant through the gastro intestinal tract, the diffusion from the food through the unstirred water layer, through the membrane and into the blood. The diffusion through the membrane was split into an inner and outer membrane resistance, where KOW reflected partitioning from the water into the outer membrane, and hydrogen bond donor strength reflected the

partitioning from the outer into the inner membrane. The model was calibrated to two data sets which were merged: uptake efficiency of environmental pollutants measured in different mammals during feeding studies, and a pharmaceutical data set with human oral absorption efficiencies.
The new model estimated uptake efficiency for compounds with logKOW ranging from -10 to +8, and estimation was improved for polar compounds by accounting for the bilayer structure of the membrane. Including the inner membrane resistance improved RMSE especially for the compounds with KOW<0 from 28.3 to 18.3, while also overall performance improved from 18.4 to 14.0. Therefore, the new model provides a tool to estimate uptake efficiency for new compounds based on sound mechanistic processes.

MO 063
A standardized contact transfer method for assessing soil-to-clothing exposure to soil-sorbed chemicals
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Exposure to chemicals, including chemical warfare agents (CWA), can present a potential Contact Hazard even when the compounds are sorbed onto soil. Previous studies have investigated levels of CWA transferred from contaminated surfaces utilizing a malleable latex material (dental dam; DD) as transfer substrate; however DD is typically inconsistent in compositions, and not reliable for toxicological investigations. Measurements of CWA on standard Army Combat Uniform (ACU), plus toxicological effects of CWA, have been reliably established for some CWA and ongoing-testing continues for others; but need still existed for a reliable transfer-exposure method for assessing the exposure potential for chemicals sorbed onto soil. We have established a method for reliably determining Contact Transfer of compounds from soil directly onto clothing, utilizing standard mass (x Gravity) as a standard force to produce a standard measure of exposure potential. We initially determined the effects of contact time and applied mass (DD); then in benchmark investigations, we established the efficacy of CWA extraction from ACU (and DD), and Contact Transfer of CWA from soil onto clothing (ACU). A 4"-diameter circular swatch of ACU material was selected, similar to surface areas that may contact soil at knee or elbow locations; standard contact was created by placing the ACU swatch directly onto the soil-surface one minute after CWA dissemination, then covering the swatch with a 4"-diameter Plexiglass disk to distribute force from a centrally-placed standard mass. Contact Transfer of CWA was determined by solvent extraction of swatches, with subsequent analyses by GC/GC-MS or HPLC/HPLC-MS. Masses 0.250, 0.500, 1.000, 1.500 kg, resulted in significantly greater CWA transfer ($p \leq 0.05$) at ≥0.500kg compared to 0.250kg; therefore the 1-kg standard mass was selected for integration into the method. Although the quantities of soil-sorbed CWA that transferred increased as a function of contact time, the rate of transfer decreased dramatically after 1h; therefore 0.25h was selected for integration into the method. The quantities of CWA transferred from soil surfaces contaminated at operationally important levels from Soil-to-Clothing (ACU) are amounts that are within the range of concern for Soldiers. The standardized Contact Transfer Method provides reliable standard predictions of exposure potential, and in conjunction with toxicity data, for predictions of Contact Hazard.

MO 064
Combined modelling of PAH biodegradation, soil sorption and dissolution from organic phases
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Despite promising microbial degradation of polyaromatic hydrocarbons (PAH) in the laboratory, pilot-scale investigations and observations at the field scale often reveal the formation of a considerable residual fraction of PAHs in soil, which is not further degraded. Non-bioavailability of PAH due to adsorption and sequestration would thus result in residual fractions resistant to microbial degradation, which may increase with time. However, residual concentrations may also be due to kinetic reasons, i.e. the concentrations may be too low to maintain microbial metabolism. For a range of biodegradation experiments, combined modelling of microbial growth and degradation, ad/desorption processes as well as dissolution from the organic phase has been carried out. The objective of the present study was to analyse and explain observed processes mathematically.
In experiments with phenanthrene added to solution as microcrystals and the degrader microbe Novosphingobium pentaromativorans, fast degradation took place at the beginning, corresponding to a strong initial increase in microbial mass. Experiments with higher initial concentrations revealed slower degradation. An initial set of Monod parameters could be fitted and experimental observations could be explained by a decreasing effective surface area for phenanthrene dissolution of the phenanthrene crystal phase. These effects were stronger with higher initial concentrations (assumed higher coagulation of microcrystals with time).
Other experiments considered were done with phenanthrene-spiked soil amendments (radio-labelled 14C-phenanthrene) in suspension and degrader strain Sphingomonas sp. 10-1 (see also Marchal et al. session C07). Biodegradation proceeded rapidly due to high cell densities of degrader bacteria. No bacterial growth, but rather a slow decline was observed. Desorption velocities could be fitted for the experiments, reflecting differences in surface areas of the soil amendments. The modelling revealed that high sorption did not have an inhibitory effect on phenanthrene biodegradation. Indeed, simulations showed that no growth of degrader bacteria was required for degradation, since the initial bacterial numbers were high enough to achieve complete mineralisation within the experiment duration. The evaluation and modelling of new experiments with different soil suspensions and added soil amendments (activated charcoal, biochar and compost) is currently under way.

MO 065
Extended dynamic range, high precision analysis of Polynuclear Aromatic Hydrocarbon compounds by GC-MS
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Polynuclear aromatic hydrocarbons (PAH) are a class of compounds used in the determination of contamination from fuels and oils and also monitored in the environment and food supply as potentially toxic compounds. The concentration range of PAHs in any given set of samples, depending on source, may be in the sub-ppb range up through the ppm range. A methodology is demonstrated which takes advantage of both GC-MS injection techniques and mass analysis techniques to extend the dynamic range of PAH analysis to encompass these concentrations. This is accomplished while maintaining the required levels of calibration, replicate and sample QA/QC (precision and accuracy), improving the productivity of the laboratory across a wide range of projects.

MO 066
Modelling PAH bioaccumulation in Mytilus galloprovincialis with a three-compartment model
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Polycyclic aromatic hydrocarbons (PAHs) are important organic pollutants in the aquatic environment due to their persistence and accumulation potential both in organisms and in sediment. With the entrance of PAHs into a clean ecosystem, indigenous aquatic biota may be affected due to the accumulation of PAHs in their adipose tissues. Bioaccumulation of pollutants may occur at each link in aquatic food chains, starting from primary producers to humans consuming various aquatic organisms with their diet. In this study, mussels were selected as biological indicators due to their broad geographic distribution, immobility and low enzyme activity, which cause significant bioaccumulation of pollutants in their tissues. PAH bioaccumulation and depuration in *Mytilus galloprovincialis* under dynamic environmental conditions were described using a three compartment model. First order kinetic equations were used for the description of accumulation and depuration of selected PAHs in mussel tissues. Data were obtained from experiments performed with selected PAHs under constant conditions. In the model, three compartments were defined: (1) mussels, (2) surrounding environment (seawater), and (3) algae (*Phaeodactylum tricornutum*) as food source for the mussels. During the bioaccumulation period, the mussels take up the contaminants both from seawater and with PAH exposed algae. Thus, the model considers dynamic exchange of PAHs between algae and seawater. Experimental data were used to parametrise and calibrate the proposed model for benzo(a)anthracene and phenanthrene. The observed dynamics could be described well for three different PAH concentrations. The model provides a mathematical description of bioaccumulation and depuration kinetics of PAHs in mussel species. For better agreement of simulation results with the experimental data, still a deeper understanding of the processes determining the chemical fate of PAH in the system of seawater, algae and mussels is required to be integrated into the model equations.

MO 067
Mass balance of polycyclic synthetic musks using a new dynamic segmented surface water/soil model
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Polycyclic synthetic musks (PCMs) are used as fragrances in a wide variety of personal care products. Among these compounds, the most important are galaxolide (HHCB) and tonalide (AHTN), used respectively, in Europe during the year 2000, at amounts of 1473 and 358 t. Since the removal of these substances through municipal sewage treatment has been estimated to be not higher than 60%, concentrations ranging from ng/L to µg/L of HHCB and AHTN are often measured in aquatic environments, posing a serious concern for ecosystems given the high potential for bioaccumulation of these chemicals. In this context, determining the exposure levels of ecosystems to these substances becomes a priority and environmental fate models represent an essential tool given the lack of monitoring data. In 2010, a survey along the Molgora River, flowing for about 40 km in a densely populated area in the Lombardy Region, northern Italy, was started. Samples of water and suspended solids were collected seasonally in 7 monitoring stations located up- and downstream of the 3 sewage treatment plants (STPs) present along the river. Seasonality in concentrations was observed, with the highest levels occurring in spring. Moreover, the samples collected downstream of the 3 STPs showed the highest concentrations. In order to investigate the reasons of this variability and to predict future trends, a new dynamic modelling approach (DynANet) based on an existing water-sediment model (DynA) was applied. In DynANet, the implementation of geographic information system (GIS) tools allows the subdivision of a river drainage basin in sub-basins and the resulting river links, classified according to the Strahler stream order, communicate by means of a downstream water flow. The loading data of runoff water and modelled chemical concentration coming from the different sub-basins are provided by the connection with the existing dynamic model SoilPlus, developed to evaluate the fate of organic chemicals in the air, litter and soil compartments and working in a GIS environment. The application of the DynANet model to the case study allowed to compile a preliminary mass balance for HHCB and AHTN and to predict concentration changes under environmental phenomena such as precipitations events, temperature variations, soil use, etc. The measured concentrations and simulated results were compared to the prediction of existing models such as GREATER.

MO 068

Estimating chemical emissions from home and personal care products in Asia

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Asia's economy is growing significantly with China and India leading the growth. This has led to an increased demand for home and personal care (HPC) products. Information on the use and sales of HPC products is critical to estimating emissions and predicted environmental concentrations (PECs). It has also been demonstrated that by coupling population density data with sales data it is possible to estimate HPC product consumption. To date, most studies have been based in developed markets, where wealth distributions are more homogeneous and HPC products are affordable to all resulting in usage being evenly distributed across the population. In Asia, a population's wealth and ability to buy HPC products is not uniformly distributed, therefore combining information on population density and sales data with a sub-population's ability to purchase HPC products could improve chemical emission estimates. Global datasets were sourced for population and economic activity incorporating population, night-time light satellite imagery and land cover. Coupling these datasets with sales data of different HPC products at a (sub) country level and 'takeoff values', (a populations ability to purchase HPC products based on their per capita GDP), emission estimates were calculated. Results show large variation in HPC product usage exist across Asia due to the variability in population density and wealth. The largest refinement of emission estimates are associated with products requiring greater purchasing power. As wealth evens out, for example the per capita GDP is above $10,000, population density becomes the appropriate method for distributing product use. The potential benefits of this approach include more accurate estimation of chemical emission patterns, which could be used to parameterise exposure models for use in environmental risk assessment and contextualising existing monitoring data.

MO 069

Chemical fate and risk assessment at large scale based on direct and inverse modeling approaches and pan-European datasets

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The chemical fate and risk assessment at large scale is typically performed on the basis of explicit GIS fate models which in turn make use of either a "direct"or an "inverse"modeling approach with the direct being a traditional one.
The direct models are based on a priori available information about chemical emissions and are intended to answer the question: "Where do chemicals go after being emitted?". Thus, when data for emissions and substance's physico-chemical properties could be retrieved from existing databases, the model predictions of spatial distribution of chemicals prove to be sufficiently accurate for screening purposes.
Oppositely, the inverse modeling deals with the question "where do pollutants come from?"and is based on measurements of chemical concentrations. Then, the inverse models may support large scale assessment, in particulare for the surface water quality by estimating chemical emission factors at regional, river basin or continental scale in relation to the population density or another apropriate proxy.
This work presents the potential of the European version of MAPPE (Multimedia Assessment of Pollutant Pathways in Environment) direct model to simulate a steady-state spreading of pollutants emitted from point or diffuse sources. The model outcome consists of annual fate maps of chemical concentrations, deposition rates, fluxes to other environmental compartments, and could be used for screening of hazard zones at continental scale with spatial resolution 1 km2. In this model exercise the target contaminants were few POPs as PCBs, dioxins, furans, pesticides, etc.
In addition the study encouraged the applicability of the inverse modeling technique for pollutants with poor and sparse emission estimates but which were extensively monitored in pan-European campaigns. As examples, the capability of the inverse GIS applications was utilised for backward tracking of PFOS and PFOA emission factors from riverine measurements and to investigate the loading of the widely used pharmaceuticals and personal care products to European rivers.

MO 070

Multimedia assessment of chemical exposure by MAPPE-Global explicit model: a case study of pollutant discharge to Mediterranean Sea

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The work describes a case study of pollutant discharge to Mediterranean Sea by a spatially explicit fate and exposure model with worldwide coverage for Multimedia Assessment of Pollutant Pathways in the Environment (MAPPE Global). The model computes removal rates of a substance with given physico-chemical properties in an evaluative environment composed of atmosphere, soil, inland and sea water, in the form of global maps with a spatial resolution of 1°x1° for air and oceans and 0.08°x0.08° for soil and surface water.
The maps of removal rates enable the computation of concentrations from known emissions in one or more environmental compartments using a simple box model, except for the stream network where a plug flow scheme is adopted. To estimate the chemical removal rates the model accounts the following elimination processes: chemical degradation; advective transport; diffusive transport; and sinking.
However, MAPPE Global does not explicitly compute chemical transport in space, but only the fate of a substance at each location by calculating chemical's mass fluxes that are available for transport outside of cells. In order to resolve this problem an adjustment procedure has been adopted comparing the Global model outcome with the results of the European version of the MAPPE model.
Then, in relation to the Marine Strategy Framework Directive and HORIZON 2020 initiative for Mediterranean Sea, MAPPE-Global was used to estimate of chemical load of a few POPs (as PCBs, Lindane, etc.) from emissions in the surrounding countries of Europe, Northern Africa and Asia. The Mediterranean Sea load assessments also accounted for the contribution of the LRAT by emission sources originated from North America or South East Asia.

MO 071

The impact of including ice and snow in multicompartmental modelling of persistent organic pollutants' distributions and fate

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Persistent organic pollutants (POPs) are multicompartmental substances. Ice or snow compartments have only recently been included in POP cycling in large scale multicompartmental modelling.
The impact of including ice and snow compartments on model-predicted distribution and fate was studied using the global multicompartment chemistry-transport model MPI-MCTM [1], which is based on a coupled atmosphere-ocean general circulation model. 10 fictive years of DDT and γ-hexachlorocyclohexane (γ-HCH) as applied in global agriculture in 1980 fate and transport under present-day climate were simulated with and without the compartments sea ice, land ice and land snow [2-3].
7-9% of the burden of the surface ocean of γ-HCH and DDT are stored in sea ice. Neglect of the role of sea ice would largely underestimate γ-HCH in surface seawater (-62% globally, -30% in the Arctic), but overestimate DDT in surface seawater (+19% globally, +107% in the Arctic). The compartmental distribution shift exceeds the mass of γ-HCH and DDT stored in sea ice by a factor of ca. 8 and ca. 15, respectively. Ocean surface waters in the sea ice melting zone receive a seasonal (summer) contamination wave which on the regional scale may double exposure.
Within 10 years 3.34% and 1.84% of the global total environmental burden of γ-HCH and DDT, respectively, are stored in glaciers over Antarctica and Greenland. Land snow is primarily present in northern winter and stores up to 0.82% (γ-HCH) and 0.45% (DDT) of the total contaminants' burden. Melting snow causes a seasonal contamination wave with a volatilisation peak and a release of pollutants to underlying soil and vegetation. The neglect of land ice and land snow in the model would underestimate the total burdens of γ-HCH and DDT stored in the Arctic (by 7% and 2%, respectively) and Antarctic (by 44% and 32%, respectively) and would overestimate Antarctic oceanic burden (by 44% and 29%, respectively).
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MO 072

Global fractionation of PCBs

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PCBs are ubiquitous environmental pollutants which are expected to decline in abiotic environmental media in response to decreasing primary emissions since the 1970s. A coupled atmosphere-ocean general circulation model with embedded dynamic sub-models for atmospheric aerosols and the marine biogeochemistry and air-surface exchange processes to soils, vegetation and the cryosphere [1-3] is used to study the transport and fate of four congeners (3-7 Cl atoms) 1950-2010.
The geographic distribution of the PCB mixture evolves over time reflecting the sources and sinks' evolvement over time. Globally, secondary emissions are on the long term increasingly gaining importance over primary emissions. They are most important for congeners of medium hydrophobicity (5-6 Cl atoms). Congeners' fractionation is characterized both geographically and temporally. It causes enrichment of the lighter congeners and more delayed decreasing levels in high latitudes in response to decreasing emissions. Delivery of contaminants to high latitudes is predicted to be more efficient than previously suggested.
The results suggest that the effectiveness of emission control measures may significantly vary among substances, not only reflected as latitudinal gradients, but also as longitudinal gradients.
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circulation model. Chemosphere 76:1509-1517.
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MO 073

Predicting the removal of atmospheric particles by vegetation with a dynamic multimedia model

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It is well known that vegetation is capable of capturing contaminants from air. In particular, plant leaves can act as a biological filter and as a sink for airborne particles and their associated Semi Volatile Organic Compounds (SVOCs) such as Polycyclic Aromatic Hydrocarbons (PAHs), influencing their environmental fate. In order to assess the filtration performance of plants with respect to atmospheric particulate matter (PM) and their associated SVOCs, deposition on vegetation has recently been investigated by a number of different methods (field, laboratory studies as well as modelling approaches). Some authors studied the particulate matter uptake and retention capacity of different plant species, showing that some plant type are much more efficient than other at collecting particulate matter and PAHs contained upon them. Other researches were focused on measuring particle deposition velocities not only for specific tree species but also at different wind speeds. Furthermore different predictive approaches were developed to evaluate PM uptake by trees in urban areas and to estimate dry particle matter deposition on leaf surfaces using species-specific deposition velocity. Nevertheless, the existing multimedia fate models do not generally account for PM mass balance in predicting PM deposition to vegetation and the corresponding chemical flux. In the present study we used a dynamic multimedia fate model (SoilPlusVeg), which incorporates a vegetation compartment, to calculate leaf particle-bound PAHs uptake from air. In this model, formulated in terms of fugacity, the vegetation compartment can be composed by a mono- or multi- specific forest canopy, which interacts with dynamic air and the soil compartments. The model, which incorporates some forest structural parameters such as specific leaf area (SLA) and leaf area index (LAI), was modified to account for some of recent findings concerning the particulate matter uptake by vegetation. Simulations were performed for some high molecular weight PAHs, as they exist predominantly in the particulate phase, for a multi-specific semi-urban wood located in Como. The results were compared to data measured in air, deposition and vegetation in the same location.

MO 074

Climatic, biological and land cover controls on the exchange of gas phase semivolatile chemical pollutants between forest canopies and the atmosphere

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An eco-physiological model of a structured broad-leaved forest canopy was coupled to a chemical fate model of the air-canopy exchange of gaseous semivolatile chemicals to dynamically assess the short-term air-canopy exchange and the influence of biological, climatic and land cover drivers on the canopy capacity of accumulating pollutants from the atmosphere. The chemical fate model accounts for effects of short-term variations in air temperature, wind speed, stomatal opening and leaf energy balance, all as a function of layer in the canopy. The model also includes a new wet deposition scheme that estimates the interception of gases dissolved in rain as a function of depth in the canopy. Simulations showed the potential occurrence of intense short/medium term re-emission of pollutants having Log(Koa) up to 10.7 from the canopy as a result of environmental forcing. In addition, relatively small inter-annual variations in seasonally-averaged air temperature, canopy biomass and precipitation can produce relevant changes in the canopy storage capacity for the chemicals, suggesting that climate change may play a significant role in determining the effectiveness of forests in controlling atmospheric transport of semivolatile pollutants.

MO 075

Assessing and comparing the influences of uncertainty in chemical property data and variability in climate variables on the simulated fate of PCBs

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Legacy persistent organic pollutants (POPs) are of concern due to their persistence, bioaccumulation potential, toxicity and ubiquitous presence in the natural environment. Environmental fate modellers have made numerous efforts to simulate the transport and fate of legacy POPs at different spatial and temporal scales. The success of modelling exercises depends largely on the quality of model input data for characterizing either the modelled chemicals or the modelled environment, e.g. the physical-chemical properties and environmental (including climate) variables. The purpose of this study is to explicitly assess and compare the influences which are caused by the uncertainty in chemical property data and variability in climate variables. Representative polychlorinated biphenyl (PCB) congeners having a range of physical-chemical proerties are selected as study chemicals. The scientific literature was mined to describe the uncertainty in the physical-chemical properties of the selcted PCBs, and online climate databases were surveyed to derive the long-term averages and projected deviations for the selected climate variables. The ChemCAN spreadsheet model is reparameterized for Japan and used to test the hypothesis that property uncertainty has more influence on model outcomes than climate varibability. The robust statistical tool Oracle® Crystal Ball (Fusion edition, 11.1.1.1.0) is adopted to perform the correlation and sensitivity analysis. Generally speaking, results suggest that uncertainty in physical-chemical property data leads to more pronounced variances in the model predictions than variability in climate variables, i.e., the predicted environmental fate and distribution of selected PCB congeners is more sensitive to uncertain physical-chemical properties than to climate varaibles. The large uncertainties associated with half-times for degradation in air, water and soil dominate influences on the model simulated fate and distribution of selected PCBs, if compared to climate variables and the physical-chemical properties. Among climate variables, temperature and its projected future deviations is the most influential. We conclude that predicting the influence of climate on chemical transport and fate is challenging due to the fact that climate-related effects on transport and fate are relatively small compared to uncertainties in physical-chemical properties and degradation rates.

MO 076

Environmental fate, latitudinal distribution and long range transport of decamethylcyclopentasiloxane (D5) in the global environment: a model assessment

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Decamethycyclopentasiloxane (D5) is widely used as an ingredient in the formulation of personal care products, or is present as an impurity in the silicone fluids and rubbers. The global environmental fate, latitudinal distribution, and long range transport of D5 was analyzed by two multimedia chemical fate models using the best available physicochemical properties as inputs and known persistent organic pollutants (POPs) as reference. The global transport and accumulation characteristics of D5 differ from those of typical POPs in three significant ways. First, a large fraction of the released D5 tends to become airborne and is removed from the global environment by degradation in air, whereas known POPs have a tendency to be distributed and persistent in all media. Secondly, although D5 can travel a substantial distance in the atmosphere, it has little potential for deposition to surface media in remote regions. This contrasts with a deposition potential of known POPs that exceeds that of D5 by at least 4 orders of magnitude. Thirdly, D5 has a short global residence time with the majority of the global mass removed within three months of the end of release. Global residence times of POPs on the other hand are in years.

MO 077

Environmental fate of D5 Predicted by the QWASI Fugacity model

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Due to the unique characteristic property of decamethylcyclopentasiloxane (D5), airborne D5 remains in the compartment until it is oxidized by OH radicals. In contrast, when D5 is released to water, multiple processes including volatilization, sorption to sediment, advection and hydrolysis take place competitively. Importantly, the rates of transport and transformation processes are dependent on the local aquatic environment. Since a better quantitative assessment on the fate, distribution and transport of D5 in a real water body system is needed, this study evaluated the environmental behavior of D5 in Lake Ontario (LO) and Lake Pepin (LP) at various environmental temperatures and under steady-state and unsteady-state conditions. Additionally, uncertainty analyses were performed to determine the most probable range of the model outcome and the most influential input parameters using a new Quantitative Water Air Sediment Interaction (QWASI)-Excel model.
The QWASI-Excel model predicted that water concentration of D5 decreased for both lakes due to increase in hydrolysis rate with rising temperatures from 1 to 25°C. In contrast, D5 concentration profiles in sediment were different: it decreased gradually from 1.0 to 0.5 ng/g dw in LO whereas it increased from 120 to 280 ng/g dw in LP. D5 mass preferentially distributed to water in LO but to sediment in LP. Mass fraction of D5 increased with temperature for both lakes mainly due to increased K_{OC} value. D5 was removed via hydrolysis and volatilization in LO whereas via advection and hydrolysis (at only high temperature) in LP. Residence time of D5 in water was relatively short for both lakes whereas residence time of D5 in sediment was much longer due to slow degradation. In contrast with a relatively short response time in water, response time in sediment was relatively long.
Uncertainty analyses with Monte Carlo simulation determined that hydrolysis half-life in water and sediment layer depth was the most influential input parameter to environmental behaviors of D5 in LO and LP, respectively. In addition, other factors such as K_{OC}, hydrolysis half-life, solid deposition rated and sediment resuspension rate also contributed to the total variations in environmental behaviors of D5 in LP. The analysis also predicted 95% confidence intervals for D5 concentrations in water and sediment, mass distribution, intermedia transport and transformation rates, residence time and response time in both lakes.

MO 078

Modelling aluminium fate and transport in ground and surface water for Life Cycle Assessment

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In assessment of the fate, transport, and ultimate exposure of metals to humans, correctly accounting for long-term groundwater emissions, e.g., from a landfill, has been challenging. This research offers a new perspective on human exposure to anthropogenic metal emissions to ground and surface water. Existing models, such as the Ecoinvent LCA database have assumed 100% of landfill emissions reach surface water. To accurately reflect geochemical and hydrologic processes, this conservative assumption can be reassessed.
A multi-component model was developed to assess the total intake by humans of emissions to landfills (for aluminum) and directly to surface water (for arsenic from aluminum ore). For landfill emissions, a kinetic precipitation model was developed to estimate transfer to surface water. In surface water, the geochemical model PHREEQC

[1], including an implementation of WHAM VI [2], was used to estimate speciation, as well as the potential for precipitation, sorption, and complexation, while hydrological data at the continental level provided estimates of continental flows and residence times. Information at the national level on drinking water source and treatment were aggregated to the continent scale and included in the model, thus providing estimates of the population fraction drinking treated and untreated ground and surface waters. Finally, speciation was used to assess bioavailability of ingested aluminum to humans.
The model shows lower estimates of transport from source to receptor than previous studies, which lacked a precipitation module. Uncertainty in input data and modeling assumptions, which will be discussed, allow the model to be applied to large-scale systems as a comparative tool. For example, the ingested intake fraction for aluminum emissions to landfills is lower than previous models by a factor of 1x106 or more, depending on the location. The continent of emission, via its hydrology and the fraction of treated / untreated drinking water, plays an important role.
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MO 079
Dioxin Source to Ecological Receptor Region HYSPLIT-SV Modeling in Mexico with Atmospheric Measurements 2008-2010: Montes Azules, Celestun and Monterrey
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Instituto Nacional de Ecología (INE) sampled and measured dioxin in the atmosphere at 10 research stations in Mexico from 2008-2010 with the support of the U.S. Environmental Protection Agency, Environment Canada, Health Canada, and the Commission for Environmental Cooperation for North America. We focus in this presentation on three receptor regions with air monitoring stations with variations in measurements that need to be explained: Montes Azules, (ecosensitive biodiverse ecoservice region, land), Celestun (ecosensitive biodiverse ecoservice, land and marine), and Monterrey (urban and agricultural). The Hybrid Single Particle Lagrangian Integrated Trajectory Semi-Volatile experimental research atmospheric dispersion model (HYSPLIT-SV) is employed to account for variations from meteorology under conditions of uncertain source emissions.
HYSPLIT-SV is a dynamic atmospheric dispersion model adapted to include atmospheric chemistry and environmental fate processes including vapor-particle partitioning, degradation (e.g. via hydroxyl radical, ozone, photolysis) and deposition (wet and dry; gas and particle). Source-to-receptor simulations produce estimates of the efficiency of transport to a receptor as air concentrations and deposition, as fractions, which we call Air Transfer Coefficients [ATC]. ATCs integrate the effects of meteorology and environmental fate processes from individual sources to selected receptors. ATCs enable the development of estimates of source-to-receptor transport under conditions of changing and uncertain emission scenarios.
Secretary of Environment and Natural Resources (SEMERNAT) and INE are in the process of developing a dioxin emission inventory in cooperation with the United Nations Environmental Program (UNEP) under the Stockholm Convention. The UNEP dioxin toolkit provides emission factors in aggregate TEQ, but not by congener. Dioxin modeling must be conducted on a congener basis, since congeners vary in physical-chemical properties that determine environmental fate processes. For this presentation, we estimate congener emissions from congener profiles based on U.S. and Canada measurements. We focus on the major point sources that have been best characterized at this time in Mexico. HYSPLIT-SV modeling output provides data that can be used to rank the importance of each source contribution to the loading to ecological receptor regions useful for efficiently targeting mitigation by policy makers.

MO 080
Mathematical modeling of point source pollutants fate and transport in the Little Akaki River, Ethiopia
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Computer models are becoming increasingly important tools in every environmental management aspects. A general one-dimensional water quality model has been developed for one of the most industrially concentrated and polluted rivers in Ethiopia - the Little Akaki River. The study covers a total of 27.4 km length along the river where pollution issues are significant. The spatial and seasonal variation of hydro-geometric properties that affect mixing and transport of chemicals in the river were estimated by correlating the river hydro-geometry in a power law model. For this purpose, 20 locations were systematically selected and field data were collected for five months. The river has been conceptualized as 1370 equal length completely mixed computational elements, and a functional representation that includes mass transport and hydrodynamic equations were written for each computational elements. The general one-dimensional model equation was solved using the numerical technique by finite volume spatial discritization and finite difference temporal discritaization. Computational solution procedures were prepared by writing a computer program code using the MATLAB programming platform (version 7.0). BOD and DO were selected as water quality indicators, and sensitive model parameters that affect fate and transport of DO and BOD in the river were calibrated. The performance of the calibrated model in predicting data not used during calibration was also estimated and the result was in good agreement with these targeted water quality data. The applicability of this model as decision making tool for pollution control activities was also assessed and the result is encouraging. Recommendation, which takes into account the existing water quality problem in the study area, has been suggested for improvement and wider application the model.

MO 081
A study of the relevance of regionalization and archetype approach for aquatic freshwater ecotoxicity
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The importance of regionalization for the aquatic freshwater ecotoxicity impact category has been evaluated at different resolutions (at a watershed, country and continental scale) using multimedia fate and exposure models such as IMPACT World, Europe single zone and Europe spatial models.
A first comparison of water fate factors between the IMPACT Europe single zone model vs. the IMPACT Europe spatial model has been performed considering both a uniform emissions and emissions in each specific watershed. Moreover three watersheds with short, medium and high residence time of water to the sea have been selected to analyze the importance of chemical properties vs. watershed specific properties to identify the key parameter(s) influencing the fate. The water residence time was used as the basis for defining 2 watershed archetypes, i.e. upstream (with water residence time >0.1 [yr]) and downstream of a lake (water residence time <0.1 [yr]). The fate factors of chemicals emitted into water calculated with this latter approach have been compared to the spatial model and differences with the a-spatial approach discussed.
The results of IMPACT World and Europe showed that a-spatial models might overestimate the chemical fate and characterization factors for fresh water ecotoxicity up to a factor 5 when compared to a spatially differentiated model for unknown emission location (i.e. assumed being uniformly emitted compared over the whole model surface). When the emission location is known, a spatially differentiated model can improve the model accuracy up to 2-3 orders of magnitude, because of its ability to accurately predict the water residence time to the sea (or out of the system) depending on the emission location. Is therefore spatial differentiation always required? The answer depends on the physico-chemical property of the chemical: only for persistent chemicals the water residence time plays a key role in determining the chemical fate for freshwater ecosystem. Highly degradable or volatile chemicals for example would disappear before being advected out of the system. This support that, for persistent chemicals, the country/ regional differentiation is relevant.

MO 082
Mixing zones modeling in the water framework directive: comparison between 'discharge test' and 'CORMIX'
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The Priority substance Directive 2008/105/EC has defined EQSs for 33 priority substances. Compliance with these EQSs should be achieved at the point of discharge or at least at the edge of the mixing zone in the receiving waters. Considering this, a "Tiered Approach"has been developed to assess whether compliance with the EQS values is achieved. The approach starts with simple investigations but could end with very detailed assessments on the mixing behavior and concentration profile of effluents in the surface waters. In contrast to lower tiers, higher tiers require an estimate of the extent of EQS exceedence that can be used to define a mixing zone. This may be achieved using a range of tools such as "Discharge Test"or "CORMIX". The aim of this presentation is to discuss the application range of both "Discharge Test"and "CORMIX". "Discharge Test"is a freely available model developed to assess the acceptability of mixing zones resulting from discharges into surface waters at Tier 2 level. This model is based on Fischer equations and requires a limited set of parameters and allows for quick modeling of effluent concentrations from single port submerged pipes only. Moreover, it ignores the importance of boundary interaction in the near field and the possibility of density current formation after initial jet/plume mixing. "CORMIX"is a USEPA supported model that can be used for Tier 2 and higher. It is a mixing zone expert system that classifies momentum and buoyancy of the discharge in relation to boundary interactions to accurately predict all different mixing behaviors. "CORMIX"is a well-validated model that requires just a few more input parameters. CORMIX takes into account all the weaknesses pointed out for "Discharge Test". "CORMIX"was not designed to present less worst case results, it was designed to provide the most accurate representation of the actual physical mixing process given a set of ambient and discharge conditions. The main conclusion is that "Discharge Test"is easy and free and can be used for Tier 2 assessments of single port submerged discharges. If more accurate modeling is required or if "Discharge Test"does not cover the discharge parameters, "CORMIX"could be used.

MO 083
Development of GREAT-ER 3.0, an entirely Open Source software for river and sediment exposure modeling
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GREAT-ER (Geography-referenced Regional Exposure Assessment Tool for European Rivers) is a GIS-assisted computer model for risk assessment and management of chemicals in river basins. Since the release by ECETOC of the original model in 1999 (GREAT-ER 1.0) a number of regional projects have been initiated by various organizations with the aim of exploring and expanding the different applications of the model.
To facilitate this process, the model system was reimplemented with a modular architecture and a database back-end in 2003 (GREAT-ER Desktop and GREAT-ER Web).

Over the years, the GREAT-ER model has served a worldwide user community, and currently more than 170 different scientific papers refer to the development or application of the model.
Under the sponsorship of the CEFIC-LRI programme the package has now been updated again as GREAT-ER 3.0 (2011). Most notably, the database has been replaced by the Open Source Software PostgreSQL. For the first time, the entire system can be installed without any software licence fee, and the scientific community is welcome to analyse and enhance the Free Software GREAT-ER. On the model side, GREAT-ER 3.0 now also includes a sediment extension, and the possibility to model lakes as part of a river basin.
Information on GREAT-ER and updates on different projects initiatives can be found at www.great-er.org.

MO 084
Case study using the tiered approach for mixing zone modeling in the water framework directive
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The Priority substance Directive 2008/105/EC has defined EQSs for 33 priority substances. Compliance with these EQSs should be achieved at the point of discharge or at least at the edge of the mixing zone in the receiving waters. Considering this, a "Tiered Approach"has been developed to assess whether compliance with the EQS values is achieved. The approach starts with simple investigations but could end with very detailed assessments on the mixing behavior and concentration profile of effluents in the surface waters. In contrast to lower tiers, higher tiers require an estimate of the extent of EQS exceedence that can be used to define a mixing zone. This may be achieved using a range of tools such as "Discharge Test"or "CORMIX". The aim of this poster is to present a test case using the tiered approach. An industrial site has a surface discharge with a flow rate of 1,000 m^3/d to a small river characterized by a flow rate of 18,000 m^3/d. Concentration of the contaminant of concern in the effluent ($[CoC]_{eff}$) is 50 µg/L which exceeded the EQS of the CoC in the receiving water of 20 µg/L. A point source is present, a contaminant with an EQS is present in the effluent and the $[CoC]_{eff}$ > EQS therefore triggering the initiation of the second tier. The Process Contribution (PC) is 2.63 µg/L representing 13% of the EQS after complete mixing. This is higher than the allowed 4% and therefore higher tiers should be initiated and an estimation of the extent of the mixing zone is required. Surface discharges are best modeled with CORMIX requiring input data on the discharge characteristics, effluent, and receiving water. Due to the importance of the near field interactions, both the geometry and position of the discharge has to be well defined. In this case study, the discharge is located on the left bank pointing perpendicular to the river with a local depth at discharge of 0.4 m and a slope of 5 degree. The discharge channel is 0.3 m wide and 0.3 m deep. CORMIX simulations show that at approximately 0.6 m downstream of the discharge point the [CoC] drops below the EQS. A proposed extend of the mixing zone is described in the guidance as $10*W_{river}$ which in the test case would be 20 m. Therefore the [CoC] will be below the EQS in the proposed mixing zone of 20 m and compliance is achieved.

MO 085
Source apportionment of chemicals under the WFD
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New Environmental Quality Standards (EQS) are being set under the Water Framework Directive (WFD) for a wide range of substances. Generally, the concentrations for these EQS are lower than existing values. However, the sources of many of these substances are wide ranging, particularly for metals and nutrients, with multiple diffuse and point source inputs into the aquatic environment. Where an EQS is exceeded, Programmes of Measures (PoMs) may be required to reduce inputs to the aquatic environment subject to considerations of technical infeasibility and disproportionate costs. The WFD states that compliance should, as a priority, be achieved via source control, applying the 'polluter pays principle'. To apply effective PoMs it is therefore necessary to accurately quantify sources of chemicals discharged to the environment. A review of available models has demonstrated that there are no available national scale source apportionment models. UK Water Industry Research (UKWIR) in collaboration with the Environment Agency and SEPA funded the development of a model for future river basin planning. The project comprised a number of key tasks: (1) specification and securing of national datasets, (2) generation of databases for different sector inputs (point and diffuse), (3) upgrading of the SIMCAT water quality model for monthly outputs and in-river partitioning for metals, and (4) the development of a GIS-Simcat interface for data processing and results visualisation.
The model allows prediction of loads of copper, nickel, lead, cadmium, mercury, zinc, PAHs, nitrogen, phosphorus and DEHP to a 1 km2 resolution for urban runoff, highway runoff, sewage effluent, storm tank discharges, combined sewer overflows, agricultural runoff from livestock and arable land, atmospheric deposition, septic tanks, mine water discharges, natural background erosion and industrial inputs. A series of detailed catchment scenario investigations were carried out on the Wear, Tame and Hampshire Avon catchments in the north, midlands and south of England respectively to assess the impacts of diffuse and point source phosphorus inputs in order to develop PoMs that may be considered as part of the second cycle of river basin planning.

MO 086
Persistence of petroleum hydrocarbons in seawater: modeling versus experimental results
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Hydrocarbons are a highly reduced form of carbon which provides a valuable source of energy for microorganisms. Therefore, mechanisms have evolved to degrade them, and nearly all hydrocarbons can be degraded under appropriate conditions. However, degradation of petroleum hydrocarbons in biodegradation studies is often underestimated, mainly due to the physico-chemical properties of these substances. One of these properties is their low water solubility, which results in low bioavailability to microorganisms. Biodegradation data are required by many regulatory frameworks around the world. In the persistence assessment for petroleum substances under the EU REACH regulation, biodegradation data for the major hydrocarbon classes present in these substances were used. In order to screen for persistence, aquatic half-life predictions for representative constituents were calculated using the BioHCwin module of the EPISuite v4.0 model. These predictions allowed narrowing the range of potentially persistent hydrocarbon classes and carbon ranges, thereby optimizing biodegradation testing efforts. To experimentally test biodegradation for the hydrocarbons of interest, a new experimental methodology was used which determined single hydrocarbon biodegradation in seawater. To prevent variability due to water solubility constraints, a passive dosing system using silicone tubing was used to load the seawater with the chosen hydrocarbons. Biodegradation was measured using a respirometer, which performed automated dissolved oxygen measurements in the test vessels and minimized variability due to experimental handling. Except for highly branched structures or structures with quaternary carbons, experimental results showed that in general, seawater biodegradation model predictions were overly conservative. It can be concluded that the combination of modeling results and targeted experimental data provided a complete and robust assessment of the persistence of petroleum hydrocarbons.

MO 087
Field to continental phosphorus fate and eutrophication modelling
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To date, it has been difficult to link agriculture practices with local, regional, and long-distance impacts. Using a milk-producing farm as an example, this work demonstrates the possibility for improved environmental impact analysis based on the integration of site-specific biogeochemical models, local hydrology data, and fate and impact models, linking these from the local to regional scale.
An existing process model (Manure-DNDC [1]) was extended to include phosphorus (P), and a new, global P transport model was developed. Based on site-specific information, the Manure-DNDC model calculates total phosphorus loss from the milk producing farm. Subsequently, watershed specific data is used to estimate the amount of P that reaches the local stream.
Once P is traced to local stream, is routed downstream using a newly developed approach [2] that incorporates advective transport, deposition in waterways due to physical settling and biological uptake, and removal from the water system due to water withdrawal. The environmental impact of these incremental phosphorus additions can be assessed by comparison to existing phosphorus concentrations.
Manure-DNDC was used to simulate the runoff flow, sediment yield, and P loads for two test farms. Predictions showed agreement with validation data within a factor of two, and always within one order of magnitude. The model predictions of the fate of emitted phosphorus show that total ecosystem impact, and the location of that impact, is strongly dependent on the location of emission.
In the case of emission to the Great Lakes, the long residence time of water means that the majority of impacts can occur within 200 km of the point of emission, depending on whether impacts are assumed to occur at all existing P concentrations or whether there is a threshold value. For emissions in the Mississippi watershed, ~25% of impacts occur within 50 km; ~45% occur between 50 and 200 km, and ~30% occur greater than 200 km away

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MO 088
ENM fate in freshwater through adaption of USEtox (tm)
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Engineered nanomaterials (ENMs) have in recent time received substantial attention, both in scientific and consumer circles, as these materials are introduced to a steadily increasing number of consumer products. This has led to environmental concerns on how this new material class behaves in the environment, at which concentrations

organisms are exposed to the materials and what effects these materials may have on the environment. In relation to metal-oxide engineered nanomaterials (ENMs) , as is the general case for ENMs, many environmental aspects are still unknown and/or hence not properly scientifically mapped. One approach that has not been given much attention in relation to environmental assessment of ENMs, more precisely the fate, exposure and effect modelling of metal-oxide ENM's is the application of adapted characterization modelling (ACM) and hence application of characterisation models designed for single (chemical) compound assessment e.g. the USEtoxTM model for characterisation of ENM effect potentials.
The purpose of this study is therefore to evaluate if existing characterisation model such as the USEtoxTM model can be applied for characterisation modelling of ENMs applying the principles of ACM. The primarily principle of adapted characterisation modelling relies on the recognition of the fact that nano-materials do not behave like single chemical compounds in the environment. The second principle of ACM relies on the fact that existing chemical characterisation can be applied to model hypothetical representatives for effect causing emissions such as groups of chemicals (i.e. aquivalence approaches applied to model mercury). In this study the approach taken was therefore to consider if USEtoxTM characterisation of ENMs is possible and appropriately valid. The characterisation was done by relating nano-material properties to chemical properties and hence model the nano-material as a chemical with representative fate and exposure patterns.
In the case study involatile ENM's (metal-oxides) were characterised in USEtoxTM applying adapted characterisation modelling. The result obtained indicates that with some limitations the approach is considered valid - the characterisation factors are considered uncertain relating to several facts such as lack of environmental studies on ENMs making is hard to assess the general environmental behaviour of ENMs and hence relate this environmental behaviour to similar "chemical behaviour".

MO 089
Use of multiple tracers to assess non-stationarity of hydrologic transport at the catchment scaleβ
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In this study, the use of multiple conservative tracers is proposed in order to calculate the arrival time distributions of a solute trough hydrologic transport. The variability of the climatic forcing and the heterogeneity of the vadose zone (soil properties, preferential flowpaths, evapotranspiration losses, etc.) acting as a stochastic hydrologic filter suggest non-stationary solute travel time distributions. Several travel-time based models have already been developed, but experimental validation is still lacking for this type of models. In order to establish experimental travel-time distributions, 1) temporally displaced tracer injections and 2) spatially displaced tracer injections are conducted in the hillslope of the Chamberonne river (Lausanne, Switzerland). Tracer concentrations are measured downstream both close from the injection site and at the catchment outlet in lake Geneva. In the first experiment, pulse loads of different tracers are injected at the same spot nearby the stream, in order to emphasize the effect of antecedent soil-water conditions resulting from climatic forcing and hydrologic filtering. The extent of the soil water deficit is the main trigger of non-stationarity in the arrival-time distributions. In the second experiment, the injection site consists of a long rectangular strip perpendicular to the water course, along which pulse loads of different tracers are injected at distances from the stream varying between 5 and 50 meters. In this case, simultaneous injections are emphasizing the effect of heterogeneity in the hydrological pathways under similar soil-water conditions. In both experiments, the use of multiple tracers analytically differentiable is essential in order to be able to identify the original time and location of the tracer injection. This allows to physically measure the influence of the sequence of precipitations and soil heterogeneity on solute transport travel time.

MO 090
Estimation of chemical concentrations in river compartments using a 1D numerical model for contaminant transport
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Exposure assessment is based on a reliable estimation of contaminant concentrations in the environment. In aquatic systems, contaminants are transported by water (liquid phase) as well as by suspended particulate matters (solid phase), complicating the determination of their occurrence, source and fate. We introduce here an efficient numerical model for the prediction of contaminant transport in a river network and present results of two case studies for both dissolved and particulate contaminants. The hydraulic conditions are simulated using a 1D hydrodynamic model (MAGE code), which presents very low computational times and allows for long-time simulation at a regional scale. The algorithm offers the option to represent multi-channel river systems, using a looped mesh, and artificial structures such as dams. The solute transport is computed by the resolution of the advection-diffusion equation, using the ADIS code coupled with the hydraulic model. This code permits to take interactions between chemicals into account. Finally, the transport of particulate contaminants is simulated with the help of erosion/deposition laws (TS code). Thus, sediment stocks and erosion areas can be located, which is of huge interest for the identification of contaminant accumulation areas. This numerical model can predict the fate of chemicals resulting from accidental contamination, as well as chronic contamination. In the first case study, passive tracing data (Rhodamin WT) were used to calibrate the longitudinal dispersion coefficient and to verify the model representation of a solute contamination in the Rhone River, France. The second case study focused on suspended sediment and particulate contaminants (PCBs and Hg) transport, based on data collected during dam flushing operations conducted on the Upper Rhone River. These two case studies demonstrated that the numerical model proposed can be an effective tool for determining concentration, transport and fate of contaminant in the aquatic environment (solid and liquid phases), offering a robust base for environmental exposure assessment studies.

MO 091
Emissions of anthropogenic pollutants in the Alpine areas: the GEMINA project
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Evidence of climate change has been observed at both the global and the local scales. It includes changes in surface temperatures and ice cover in the Arctic, widespread changes in precipitation pattern and amounts, ocean salinity, wind patterns and incidents of extreme weather including droughts, heavy precipitation, heat waves and intensity of tropical cyclones. Climate change influence the status of the ecosystem, that may accordingly be affecting human systems.
In this context, GEMINA, a project funded by the Ministry of Education, University and Research in Italy, aims at creating an interdisciplinary network of experts with the capability of developing climate simulations, analysing the impacts of climate change and providing developing mitigation and adaptation scenarios.
GEMINA includes also the specific objective of analysing the impacts of climate change on the fate and transport of selected anthropogenic pollutants (namely, persistent organic pollutants, POPs) in the environment, in order to identify how climate variables could affect the source-to-sink relationship into remote alpine environments.
Several multimedia fate and transport models have been applied to assess the overall POPs' persistence, long range transport and bioaccumulation, and to analyse the effect of climate change on their environmental distribution, as POPs' environmental fate and transport is a function of the climate variables (e.g. temperature, atmospheric circulation, and precipitation).
We will present a case study located in proximity to a source of POPs. The main focus is to define emission scenarios according to the Special Report on Emission Scenarios defined by the IPCC in order to identify the effect of climate change on POPs' environmental behaviour in mountainous regions.

MO 092
Bioaccessibility options for detailed quantitative risk assessment of metals
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The United Kingdom has adopted a risk based approach for the assessment of contaminated land and human health impact. As part of this approach, Soil Guideline Values (SGV) and Generic Assessment Criteria (GAC) have been developed to enable Generic Quantitative Risk Assessment (GQRA). One of the main assumptions in the derivation of these assessment criteria is that 100% of the contaminant present in the soil will be bioavailable or bioaccessible. Although this assumption may be necessary in the preliminary stages of risk assessment to ensure the protection of human receptors, it may result in overly conservative risk assessment. Recommendations for remediation may subsequently be made in situations where remediation is not appropriate.
Over recent years the potential for bioacceiblity data to be incorporated into Detailed Quantitative Risk Assessment (DQRA) has been increasingly recognised. To investigate the potential for the application of bioaccessibilty data in DQRA, GAC which incorporate published bioaccessibilty data (GAC_{BIO}) have been derived using the Contaminated Land Exposure Assessment model (CLEA). GAC_{BIO} have been derived for selected metals; arsenic, cadmium, mercury, nickel and vanadium for standard residential, commercial and allotment land uses. By comparing GAC_{BIO} to typical contaminant concentrations encountered in UK soils we explore the options for the future application of bioaccessibilty data in DQRA.
A risk evaluation of the need to remediate based on the use of literature estimates of bioavailability or of GAC that invoke generic bioavailability values would be difficult to defend. GAC_{BIO} can however be useful in deciding whether to incur the cost of site specific studies of bioavailablity. The applicability of GAC_{BIO} can be be determined by considering three lines of evidence: history of contaminant formation (natural or anthropogenic); geochemical sequential extraction and physiological based tests. The natural or anthropogenic geochemical processes that led to the formation and current dispostion of the contaminants of concern (CoC) at any specific site will give an indication of the likely chemical instability and therefore bioavailability of such CoC. Sequential extraction testing can give an indication of the mineral species with which different fractions of the CoC are associated and hence their likely availability. Finally empirical physiologically based tests can give an insight into the material specific chemistry.

MO 093
Urban versus rural GIS-based distinction for human health impacts in LCA. Application on automotive fuels
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Life cycle assessment (LCA) is frequently used to assess the sustainability of the various alternative fuels that are emerging. However, local impacts, especially human health (HH), are often neglected. This is because they are heavily dependent on the local context and thus difficult to understand. In this study, we introduce two distinctions in order to improve HH impacts in LCA of alternative fuels : urban versus rural and high versus near-ground emissions.

We assess the HH impacts associated with volatile organic compounds (VOC), particulate matter, nitrogen oxides and sulphur dioxide atmospheric emissions (main pollutants emitted by cars). To assess their impacts, two indicators are retained: USEtox (for VOCs) and ReCiPe2008 particulate matter formation potential (PMFP, for the other pollutants). Two systems are studied: internal combustion engine (ICE) cars (using gasoline and diesel fuel) and electric vehicles (represented here by a Renault Fluence ZE using power coming from hard coal and natural gas).
To assess the rural and urban parts of atmospheric emissions, a geographical information system (GIS) was developed, allowing knowing the share of urban emissions all along the life cycle of the systems studied. It is then coupled with USEtox distinction between urban and regional emissions. For PMFP, the ReCiPe methodology was coupled with the Ecosense model from the ExternE project, allowing differentiating between urban and rural emissions.
For distinction between near-ground and high emissions, the same methodology using Ecosense was applied to PMFP. For USEtox, the characteristic of the compartments, especially the mixed height of the air compartment, were modified.
Three conclusions can be drawn from the results: first, applying a rural / urban distinction has a strong effect on USEtox and PMFP results. Secondly, the high / near-ground distinction also modifies the results, especially for ICE cars. Finally, the superiority of one fuel on another is complex to assess, as we did not study all HH impacts (heavy metals emissions and photochemical ozone formation are not assessed here).
Further researches should focus on the four following points: extension of the methodology to photochemical ozone creation, extension to the whole car LCA, integration of the results with other impacts and assessment of damages (endpoint level).

MO 094
A new version of input decision for the selection of modelling endpoints for PECgw simulations for harmonisation of exposure assessment
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The EU and national registration processes require the assessment of the leaching potential of an active ingredient and its metabolite(s) of plant protection products (PPP) to groundwater as described in the FOCUS Groundwater reports (2000 and 2009). For groundwater simulations using FOCUS-PELMO 4.4.3 in the framework of the national registration procedure in Germany new recommendations related to Tier 1 and Tier 2 were published by the Federal Environment Agency (UBA) and the German Agrochemical Industry Association (IVA) (Holdt et al. 2011). Input Decision 3.1, an easy to handle MS Excel-tool, was developed to select sorption endpoints for realistic worst case groundwater modelling considering a relationship between sorption behaviour and soil properties e.g. organic carbon content (OC), pH-value or cation exchange capacity (CEC). Furthermore, a procedure has been developed to select degradation endpoints depending on a significant correlation between DT_{50}-values and soil pH-value as well as taking the variability of DT_{50}-values into account. The significance of a correlation between degradation and/or sorption behaviour and soil properties is investigated by the Kendall rank correlation test that is implemented in this tool, too. This method represents a reliable statistical test when only a few values (e.g. min. 3 to 6) are available.
Input Decision 3.1 provides:
- Clearly arranged templates for normalisation of laboratory DT_{50}-values depending on temperature and moisture of soil degradation studies using either default or measured values of soil moisture and/or temperature,
- Statistical evaluation of dependency between DT_{50}- and pH-values from laboratory soil and field degradation studies and recommendations for the selection of DT_{50}-values and the scenario,
- Statistical evaluation of dependencies between Kf/Kfoc and soil properties and recommendations for Kf/Kfoc and scenario selection.
Key benefits are the simultaneous test of significance of correlations between several substance properties and soil parameters using the Kendall rank correlation test and the derivation of modelling endpoints for DT_{50}- and Kf/Kfoc-values linked to the recommendation to apply one or two suitable scenario(s) in FOCUS-PELMO 4.4.3 simulation relevant for the German groundwater assessment. The approach presented here may contribute to a harmonisation of exposure assessment for PPP between national, zonal and European level in future.

MO 095
Estimation of soil moisture and soil temperature based on different soil hydraulic pedotransfer functions
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The time-step normalisation procedure as described by FOCUS (2006) can be used to normalise soil field dissipation rates and to derive DT50 value standardised to 20°C and pF = 2. This normalisation procedure decreases or increases individual day lengths by means of daily correction factors based on soil moisture and soil temperature. Hence, soil properties such as moisture and temperature also need to be available in daily resolution. For many soil dissipation studies in the field, these parameters are, however, not readily available. In order to still run a realistic assessment, average daily soil moisture and temperature values can be estimated with predictive models, e.g. PEARL.
For the present assessment, van Genuchten parameters are derived from the soil properties of a trial site located in Central Europe. Therefore, three different types of soil hydraulic pedotransfer functions are tested. The respective results will be compared to measured soil conditions to determine a simulation method that represents realistic field data the best. Climate data (min/max temperature, precipitation, global radiation) were available in daily resolution for the complete time-span of the study. Additionally, measured soil moisture (10 cm depth) and soil temperature values (5 cm and 20 cm depth) for 12 data points were available, respectively. Hydraulic pedotransfer functions were prepared based on the HYPRES database (Nemes et al. 2001), the Rosetta database (USDA 2000) as well as the Staring Series (Wösten et al. 1994, Van Genuchten 1980). For each approach a specific PEARL scenario was created using the corresponding van Genuchten parameters. For the PEARL simulations a soil profile of 1 m depth were defined. The profile consisted of five horizons (20 cm each). Soil characteristics were only available for the uppermost horizon (0 - 20 cm) and they were duplicated to be identical in all horizons. The PEARL soil moisture and soil temperature simulations were evaluated for the first horizon (0 - 20 cm) for different depths steps (1 cm resolution). The simulated daily soil moisture and soil temperature data from the respective depths were compared to soil moisture and soil temperature measurements from sampling dates to validate the PEARL parameterisation. Using a goodness-of-fit indicator (sum of squared errors between simulated and estimated volumetric soil moisture), the estimation method that represents measured data from the trial site the best will be determined.

MO 096
Bank filtration simulation model SiMBaFi - a tool to refine the PECgroundwater as part of the environmental risk assessment of medicinal products for human use?
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Model calculations are an important component for the exposure estimation of human pharmaceuticals within their environmental risk assessment following the EMA guideline (EMEA/CHMP/SWP/4447/00, Juni 2006). In Phase II Tier A of this guideline the potential entry of a pharmaceutical into the groundwater ($PEC_{groupdwater}$) by bank filtration is calculated by multiplying the predicted environmental concentration of surface water ($PEC_{surfacewater}$) by a factor of 0.25. This factor does not consider substance specific properties, but originated by expert judgment.
The mathematical simulation model SiMBaFi was developed in a project to replace the multiplier (0.25) by a model based decision matrix taking into account the following parameters: distance between shore-line and extraction well, depth of filter screen, hydraulic conductivity and average extraction rates. The result was a Microsoft Access application which calculates the $PEC_{groundwater}$ for 3 standard flow times scenarios (worst case = 0.15 d, realistic worst case = 5 d, median case = 100 d). The following substance specific parameters are needed as input parameters to determine the concentration in groundwater: sorption coefficient (Kd) and degradation (Dt50).
This poster will present the results of groundwater exposure calculations with SiMBaFi for more than 30 pharmaceutical ingredients for which experimental data on adsorption and degradation in a water-sediment system were available. The comparison with the multiplier allows a first assessment if an implementation in the environmental risk assessment as groundwater exposure tool is useful.

MO 097
Biofilms in heterogeneous soils: reactive transport of active substances revisited
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The heterogeneity in soils is influenced by its texture, density, porosity, and the distribution and state of microbial life. Soil physical properties as well as microbial life have an impact on the fate of active substances in the soil environment. Microorganisms occur in soil pores either in suspension or as biofilms which alter the pore geometry while growing. This alteration directly influences the soil water flow field and hence the convective transport of organic substances. Furthermore, the activity field of microorganisms degrading those substances depends on soil structure. We will present an upscaled model which combines spatial stochastic generation of soil structures at pore scale and a process model at column scale coupling fluid flow, reactive transport, and biofilm dynamics. Process models are formulated by a system of coupled partial differential equations which are solved by a Petrov Galerkin scheme (COMSOL Multiphysics); the spatial stochastic process model is based on Gaussian Random Fields (R). The model is applied to investigate the degradation behaviour of pesticides in a range of soils through variation of the degree of heterogeneity. This underlines the significance of the effect of soil structure and microbial activity field on transport and degradation of pesticides.

LC01P - Development in life cycle inventory analysis and modelling

MO 098
LCA studies of biofuels in multi-output biorefineries
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The holistic nature of Life Cycle Assessment (LCA) is becoming an indispensible feature in the assessment of sustainable development of society. It is therefore integrated more

and more in decision making, where especially the Carbon Footprint is the exponent of the increasing popularity of LCA. However, several methodological choices still cause discrepancies in the final results, where the allocation procedure is a key issue. Much can be learnt from the current situation, where different regions propose new Carbon Footprint methodologies, with their own specific methodological choices. This causes problems when incorporating LCA results, such as the greenhouse gas (GHG) savings of biofuels, in legislation. In this work, a case study is executed in a Belgian multi-output biorefinery producing a mix of food, feed and fuel. Results, calculated with a black box and subprocess approach for economical value, mass, energy and exergy allocation, show discrepancies of up to 59% between the same procedure in subprocess and black box allocation, with a factor 4.1 difference within black box allocation approaches and 1.8 within subprocess allocation. The GHG savings of the biofuel versus the fossil fuel equivalent differ from 21 to 56%. When considering a broad waste definition, as is suggested by some methodologies, GHG savings range up to 80%. This work highlights that the subprocess approach is preferred, as this reflects reality better. Furthermore, physical relationships, and especially exergy, are very useful in allocation, as economical values fluctuate in time, and can cause difficulties in finding representative values of intermediate flows in biorefineries.

MO 099
A mini-Delphi approach to consensus
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The Delphi method was originally developed as a forecasting method in which a panel of experts is used in a structured manner aiming to a common understanding. We used a version of the Delphi method to resolve a methodological problem where there is no objectively correct solution: deciding the primary energy factor of industrial waste heat, heat generated as byproduct, and heat produced from waste, when these are used for district heating in Sweden. In this context, the aim was not to find acorrect answer but to take advantage of the structured Delphi procedure, including its psychological effects, to reach consensus. Our approach was a mini-Delphi: a one-day workshop with 12 participants, representing different types of stakeholders. After an introduction to the methodological approach and to the mini-Delphi approach, the participants discussed the primary energy for the heat source in three groups to improve their understanding of the issue. Each participant then individually put a sticker on a numerical scale to represent the primary energy factor that the participants felt appropriate for the heat source discussed. When all participants did not immediately agree, the participants with the extreme values where asked to justify their decision. All participants where then allowed to revise their decision. Only one such iteration was made for each heat source due to the time constraints of the workshop. The approach yielded consensus on that waste heat should carry zero, and that heat as a byproduct should carry only primary energy corresponding to the increase in primary energy demand of the industry selling the heat. The workshop also converged on the view that waste that should not be recycled should carry zero or very little primary energy when used as fuel. Similar excercises can be performed to search for consensus in other methodological issues such as allocation of emissions from multifunction processes.

MO 100
The Cereal Unit allocation as a new allocation procedure for agricultural life cycle assessments
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Background

For agricultural life cycle assessments (LCA) several different allocation approaches are currently used. This leads to a broad range of results. In addition, parts of the environmental burden might not be accounted for, if individual products are co-produced in the same agricultural system but used in different sectors, e. g. wheat grain used in bakeries and wheat straw used in biofuel production. The users of the individual co-products (baker and biofuel producer) typically do not know of each other and as a result the allocation methods for their individual LCAs are not aligned to each other. This can lead to situation that the total environmental burden is allocated inadequately.
Material and methods
Specific requirements for a suitable allocation method for the agricultural sector are defined, which were used to identify the Cereal Unit (CU) as a promising parameter for an agricultural allocation procedure.
Results and discussion
Currently available allocation methods do not satisfy all requirements for the wide range of agricultural products. Therefore, a new allocation approach based on the Cereal Unit is suggested. The Cereal Unit has been developed since decades for purposes of agricultural statistics and is optimized continuously. It is based on physical, chemical and nutritive properties. Using the Cereal Unit conversion factors, almost all agricultural products can be allocated based on one common parameter. Exemplary results will be shown, among others, for wheat, rapeseed and sugar beet.
Conclusions and recommendations
The Cereal Unit allocation approach allows using one common allocation procedure within agricultural LCAs by meeting the requirements of this sector. This approach could help to solve agricultural allocation problems and might lead to more robust LCA results for services and products originated from agricultural raw materials. We recommend investigating the applicability of the Cereal Unit as allocation approach for agricultural LCAs.

MO 101
Life cycle analysis (LCA) applied to process, integration of process modelling in the building of life cycle inventory - example of a bio-polymer production process
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Life Cycle Assessment (LCA) methodology is a well-established analytical method to quantify environmental impacts, which has been mainly applied to products. However, it also has the potential as an analysis and design tool for processes [1]. One of the interesting identified challenges of LCA applied to processes is the consideration of the operating conditions in the building of Life Cycle Inventory. It allows taking into account unit process as complex systems instead of black boxes and considering the environmental impact of the used operating conditions. This could be then interesting in multi-objective optimization (e.g. technical, economic and environmental) of processes and help the stakeholder in decision making process at the time of scale up.
This work is based on the case study of an existing pilot process for the production of a biopolymer from wheat straw and bran. An original production process, based on twin-screw extrusion and ultrafiltration processes has been developed. A first cradle-to-gate LCA has been lead in order to help the chose into different options for unit processes and then to identify the hotspots of the process.
Then ultrafiltration process have been modeled using Excel flowsheet, and twin-screw extrusion was studied througout experimental design. Both of these tools provide inventory datas for several operating conditions and have been coupled to LCA with the aim to obtained results about the environmental impacts of each process unit depending on its operating conditions.
This approach gives new perspectives in the fields of LCA applied to process industry: instead of using the methodology as an assessment method coming at the end of the process design, these one is rather integrated at the early stage of process conception with other parameters like economics and technicals.

MO 102
Exergy analysis and LCA - a design for environment approach of energy conversion processes
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LCA has been applied widely to design for environment (DfE) of energy conversion processes. It covers the environmental impacts from fuel consumption and the construction, operation, maintenance and disposal of plant components. However, due to the methodological scope of LCA, the environmental impact is related to the product of the energy conversion process, for example to the amount of electric energy generated by a power plant. Especially the functional interdependencies between the process components are not known due to the lack of a harmonized physical base of all modelled plant components.
This gap can be closed by an exergy analysis which enables the allocation of environmental impacts to exergy streams as thermodynamical basis for the overall process. To minimize the overall environmental impacts of an energy conversion process, it is necessary to consider all sources of environmental impacts and understand their formation. A new methodological approach has been developed based on the combination of exergy analysis and LCA. The so called exergoenvironmental analysis assignes environmental impacts to exergy streams. It identifies the environmentally most relevant process components as well as possibilities for the optimization of plant components. As a case study, an energy conversion process consisting of a high temperatured solid oxide fuel cell (SOFC) integrated with an allothermal biomass gasification has been analyzed.
The investigation reveals the components which have the greatest environmental impacts caused by their thermodynamic inefficiencies and their life cycle (component-related) respectively. It is shown the distinctions between the results of the LCA and the exergoenvironmental analysis, as well as the influence of the exergy destruction on its environmental impacts.

MO 103
Hybrid approaches in life cycle assessment
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With the ultimate goal to assess the Greenhouse gas emissions of the livestock supply chain in Italy, different life-cycle based methodologies were reviewed with the aim to apply the most appropriate one. Input-Output Assessment (IOA) and Life Cycle Assessment (LCA) are two of them, which have both been applied for this specific aim. Both these methodologies have their limitations, and to try to solve some of them, Hybrid methodologies have emerged, resulting in a more complete assessment. The Hybrid methods have the advantage of incorporating the details of a product perspective given by LCA, with the completeness of the economy-wide accounting of IOA. Therefore, theoretically they are considered a promising approach for linking the micro (product) with the macro (economy-wide) level, which is the core of our goal.
Several Hybrid methodologies have been proposed, with not always a clear distinction among them. We identified three main categories, namely Tiered Hybrid Analysis (THA) applied by among other Treloar et al. (2004), Input-Output Hybrid Analysis (IOHA) reviewed by Joshi (2000) and Integrated Hybrid LCA (IHLCA) devoloped by Suh and Huppes (2005).
IOHA is the most applied followed by THA and IHLCA, in the area of energy, fuel, forest and waste. Hybrid methods have been also used for the comparison of different life cycles as organic and conventional farming techniques, and for the environmental assessment of regions and countries. When compared, Hybrid methods often show a higher emission level then LCA or IOA, explaining why they are often considered as a more complete assessment. However, this higher value can also be caused by double counting

and errors in data handling. In the same time, when comparing IHLCA to IOHA, the different methods have shown differences in results depending on the input assessed. A review of the case studies in which these approaches have been applied is presented, together with their advantages and disadvantages. Suggestions of potential applications and improvement possibilities are also discussed. If Hybrid methods are a relevant substitution to LCA and IOA, is probably too early to say. Even if some of the methods have been more applied than others, there is still many uncertainties in the results with the potential to improve them.

MO 104
Multi-demand modeling in LCA - the assessment of household consumption in Swiss communities
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Environmental consumption analyses mostly focus on countries and whole economies, because for this level economic input-output tables are available that allow for environmental extended input-output analysis, and the top-down approach guarantees that all environmentally relevant sectors are covered by the analysis. The national impacts from those studies are then often divided by the number of inhabitants to reflect average impacts per capita. However, neither do these average results allow for analysis of distribution of environmental impacts within a society, nor can they serve a basis for decision-support in a legislative processes. Only a bottom-up approach is able to fulfill such requirements.
We developed a model that is capable to assess environmental impacts of individual households by means of life cycle assessment (LCA). As this approach is heavily computational intensive, we restrict the spatial scope of the analysis to communal level. Three separate models for housing, mobility and nutrition demand, determine the consumption of synthetic households. Theses households, although synthetically generated, reflect in their entirety the statistical census data of Switzerland. The consumption data of all households is compiled in a final demand matrix. Each column of this matrix represents the final demand vector of one household. The elements of each vector describe the demand for certain reference products from the life cycle inventory (i.e. ecoinvent v2.2). As there are several thousand households in an average Swiss community, the final demand matrix consists of several thousand columns. The multi-demand LCA yields the characterization results for each household. As the households are geo-referenced, we are able to visualize of the characterization results on a map.
A case study shows that environmental impacts are not distributed equally over the evaluated community. The Gini-coefficient, a measure of statistical dispersion, for CO_2 eq. emissions is 0.35 for housing and 0.66 for mobility. This suggests that environmental impacts from housing are generated more equally than environmental impacts from mobility. The model is a promising approach to characterize the environmental performance of communities based on their inhabitants, to show graphically where highly emitting households are located, and to support local decision-makers by indicating households with big leverage potential for the reduction of environmental impacts in their community.

MO 106
LCI model based on linear programming for the optimization of regional waste management systems
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Waste management systems are commonly expected to meet numerous (and sometimes conflicting) objectives, e.g. to maximize environmental protection and resource efficiency, to minimize monetary cost, to achieve social acceptance, among others. At the same time, the degrees of freedom and type of decisions to be taken in waste management are context-driven and dependent on a variety of factors, e.g. consumption patterns, availability of technology, infrastructure and capital, and on policies and regulations. The optimization of the environmental impact of waste management considering all the aforementioned limitations and constraints imposed by the regional context is hence a challenging task that requires advanced decision-making tools.
To tackle this challenge, a systematic tool based on a rigorous mathematical programming approach was developed. The optimization problem was posed in mathematical terms as a linear programming (LP) model, comprising two main sets of equations. The first includes mass and energy flow-based process models of common treatment options, including both dedicated waste treatments and co-processing activities. These models enable the quantification of the direct emissions and the resources consumed according to the amount and type of waste to be treated and the technologies available. The second set of equations determines the life cycle inventory (LCI) of inputs and outputs associated with the system operation. The life cycle inventory can be further translated into the associated impact using a damage assessment model.
The model output is the optimal allocation of waste and resources to the available or planned waste treatment infrastructure. This allocation should ensure a given required functionality (both in terms of waste treatment and industrial productivity) while conforming to the constraints imposed by the regional context. The capabilities of the approach presented are illustrated through a case study. Numerical results highlight the importance of considering multiple objectives to avoid shifting burdens between impact categories. In addition, the environmental relevance of shadow prices, i.e. the marginal environmental impact of tight constraints, is discussed as an approach to analyze sensitivities and identify opportunities for improvements. The ultimate purpose of our tool is to guide policy makers and practitioners towards the adoption of waste management patterns with improved environmental performance.

MO 107
Material flow management of biogenic municipal waste: assessment of different technology options by means of LCA
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Currently, the German law on the collection and utilization of waste (Kreislaufwirtschafts- und Abfallgesetz (KrW-/AbfG)) is in the process of amendment to comply with the European waste legislation. One of the main goals is to ensure that any recyclable material from households is to be collected from 2015 on, including biogenic municipal waste.
Generally, biogenic municipal waste can be burned, composted or fermented. Currently, in administrative districts that do not collect biogenic municipal waste separately, the waste is burned in municipal waste incineration plants and the generated electricity and heat are supplied to public. In administrative districts with a separate collecting system the biogenic municipal waste is composted. Composting plants are the backbone and state of the art for further processing of biogenic municipal waste in Germany. The product of these composting plants is sold as fertilizer or soil enrichment to horticultural, agricultural and landscape gardening companies, retail sector or private consumers. Since most of the plants are 10 to 15 years old, they need to be upgraded. A technical possibility of upgrading includes the generation of biogas from waste. The digestate could be either used to generate compost or be burned to generate electricity and heat. Generating compost could result in an increased potential to convert energy from waste, without interfering in the established material flows of biogenic municipal waste.
The objective of the poster presentation is to present, assess and compare from an environmental point of view the current state of the art of technologies to ferment biogenic municipal waste and to use the residue as compost for German requirements. The system boundary of the assessment includes the collection of waste, the fermentation and the distribution of energy and compost.
The environmental assessment of the technologies is based on a comprehensive literature analysis. The findings of the literature study are used to develop a life cycle inventory for each technology. Furthermore a draft assessment of the environmental impacts is discussed.
The results are part of the project BioEnergieDat, whose goal is to provide a database with harmonized, validated LCI data concerning provision of bioenergy under German framework conditions. The database shall simplify assessments in the bioenergy sector and thereby accelerate decision-making processes in the government and for companies.

MO 108
Life cycle assessment of flexible power plants based on difficult fuels
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Due to the increasing share of solar and wind power generation, the load management needs flexible options to manage fluctuations in power supply as well as in power demands. To handle these fluctuations, a new kind of power plant is in development at Karlsruhe Institute of Technology. This power plant consists of a moving grate which is fairly insensitive towards the fuel input and is fired with several biogenic fuels. Additionally, a pulverized-fuel burner is implemented which is co-fired with coal/biomass and can vary the power generation within several minutes. The biogenic fuels are residues which have some disadvantages like low heating values or low ash melting temperatures. Nevertheless, these fuels are so far mostly unused and are available on a regional scale. The power plant has a planned total output power of 20 MW_e.
For this power plant, a modular LCI model has been implemented. To compare the environmental impact of this power plant concept with other options for power generation, there has to be a suitable reference system. A common reference system is the electricity mix of a country. However, to cope with a power plant concept which aims to fulfil base load and peak load demands simultaneously, a comparison with an average load structure is not a suitable option. Either, the power plant concept with the flexible burner system could be evaluated by contrasting the concept with a typical base load power plant (e.g. lignite) and a typical peak load power plant (e.g. natural gas). However, the results of such a comparison could be misleading, since the power performance of both concepts differs by a factor of 10 to 50. Or, since this power plant is still under development and will not be available until 2018-20, the future types of electricity production should be considered as well. So, to identify a suitable reference system, current as well as future ecological (environmental impacts), economic (profit) and political (e.g. independency in fuel imports, CO_2 reduction targets) aspects have to be incorporated.
The objective of the poster presentation will be
- to discuss criteria to identify an appropriate reference system
- to identify the appropriate reference system, and
- to compare the new power plant concept with other power plant concepts, by selecting different scenarios for current power plants as well as for future power plants.
The results will be presented and the environmental impacts of the new power plant concept will be discussed.

MO 109
Carbon flows from land use changes in LCA on bioenergy as a function of biomass demand and spatial allocation of land
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LCA is designed to calculate environmental impacts in relation to the functional unit, based on the assumption of a linear correlation. In the case of bioenergy, rising demand may lead to land transformation and induce additional carbon flows to the atmosphere, which are not linearly coherent. International environmental policy strategies pursue

ambitious goals regarding GHG-reduction by the bias of increasing biogenic end energy supply targets for 2020-2050. Nevertheless, the impacts of soil and vegetation carbon pools due to land use change might compromise GHG-emission savings along the entire process chain. Employing representative and prospective bioenergy scenarios for Germany as a case study within the framework of our research revealed that land use change and consequent GHG-Emissions are not correlating linearly with the level of bioenergy demand. The nonlinearity is partly accounted for by the fact that various soil and above ground vegetation contains different amounts of carbon pools. Moreover GHG-Emissions due to land use change depend on the type of land transformation that occurs and the productivity of the particular land. Hence, land use should not be modelled as a linear function of agricultural or resource output with increasing bioenergy production targets within the scope of LCA. More importantly the carbon emissions released to the atmosphere due to land use change partially overcompensated the savings by the replacement of fossil fuels. For a reliable assessment of land use change based on a specific bioenergy demand it is vital to assess the investigation on a spatial explicit level. On that account we consider coupling LCA with the land use model LandSHIFT, which is a model for simulations of spatially explicit large-scale land-use change dynamics and their environmental impacts and describes the interplay between anthropogenic and environmental system components as drivers for LUC. The model input is a set of exogenous drivers such as population and production of agricultural commodities. The model output is a time series of high resolution raster maps of the changing land use pattern that can be processed as input for LCA respectively. Based on the land use patterns that LandSHIFT generated for different bioenergy production targets we calculated the carbon flows and investigated the correlation between bioenergy demands, resulting land use change and carbon flows for German scenarios.

MO 110

Capturing spatial heterogeneity using GIS: an LCA case study of pressure management in geologic carbon sequestration

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Life cycle stages for emerging environmental impact mitigation technologies require assessments within a real-world context in order to accurately predict economic, environmental, and social impacts in LCAs. Unlike a product in circulation, emerging technologies have yet to interact with markets, environments, laws and cultures. Because LCA conclusions can strongly influence decision makers, it is critical that regional heterogeneity is captured in data used for LCA metrics and for simulating market mechanisms. Geographic Information Systems (GIS) provide an opportunity to capture regional variations. Our case study is the Lawrence Berkeley National Laboratory LCA of pressure management for geologic carbon dioxide capture and sequestration (CCS). The objective of this study is to evaluate the regional variability of economics, environmental impacts, and risks of a pressure management technique involving brine extraction. We select three saline aquifers targeted for CCS from different geographic regions in the USA to assess brine extraction and disposal scenarios. GIS databases are queried for data from those three regions to perform network analysis. Initial calculations were performed assuming ten GW-size coal fired power plants were injecting 90% of their CO2 emissions into a saline aquifer CCS site with an annual injection of nearly 90 million tonnes of CO2 and an annual brine extraction of nearly 200 million gallons. We find that impacts and the potential commercial value of brine vary substantially between regions due to differences in brine composition and in market data. Water residing in the three saline aquifers spanned a range of temperatures and compositions. Economic value was sensitive to regionally specific electricity providers, salt and mineral markets, and water scarcity. Net values for management scenarios ranged from a cost of $50/tCO2 to a return of $50/tCO2. The unexpected finding that pressure management could mitigate the cost of CCS in certain regions of the USA would not have been recognized if national averages were used in calculations. While averages may be appropriate for upstream or downstream sectors in an LCA, national average values may not be reliable to the order of magnitude required for scenario modeling. The quantification and evaluation of economic mechanisms and regionally specific market data using GIS provides a more spatially resolved alternative to current national-scale input/output economic sectors in LCA.

MO 111

On strong and poor arguments for carbon capture and utilization: an LCA perspective

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Carbon Capture and Utilization (CCU) is most often motivated using environmental ad-hoc criteria like CO_2 balances, fixation amount and fixation duration. In this work, we provide the rigorous integration of these criteria into the Life Cycle Assessment (LCA) methodology. A major driver for CCU is its climate change mitigation potential. In CCU, carbon dioxide (CO_2) is captured from large-scale CO_2-emitting sources such as fossil fueled power plants. In contrast to Carbon Capture and Storage (CCS), where the CO_2 is stored in geological formations, in CCU, the carbon is re-used as a feedstock for fuels or chemicals. The capture and subsequent utilization of the CO_2 promise reductions of both greenhouse gas (GHG) emissions and fossil fuel depletion. Up to now, CO_2 balances for the utilization process have been used as a metric to account for the amount of CO_2 fixed in carbon-containing products [1]. However, this metric does not provide any information on the actual CO_2 emissions reductions. The evaluation of these reductions must account for the entire life cycle from cradle to grave. In particular, upstream processes such as the CO_2 capture process have to be included; therefore, the use of Life Cycle Assessment (LCA) is mandatory. Yet, potential pitfalls and methodological limitations exist in the application of LCA to CCU: the CO_2 capture effect is easily misevaluated; the CCU system is inherently multi-functional; and the important criterion of CO_2 fixation duration is not considered in a static, attributional LCA. This work shows how the pitfalls and limitations can be overcome to achieve a sound assessment of the environmental impacts of CCU.

MO 112

Utilization of CO2 captured in coal power plants for photocatalytic methanol production - ecological implications

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One way to reduce climate-related CO_2 emissions from coal fired power plants is carbon capture and storage. Another possibility could be the use of CO_2 captured as a secondary feedstock for a photocatalytical conversion to methanol. Such a process is developed within the research project "Solar2Fuel"(funded by the German Federal Ministry of Education and Research), clarifying technical requirements, economic conditions and ecological effects. The conversion envisaged takes place within a photocatalytical reactor using dye-sensitized catalysts, which encourage the overall equation $CO_2 + 2\ H_2O$ + solar energy --> $CH_3OH + 1.5\ O_2$.
This study evaluates the energetic and ecological prospects of the photocatalytical concept (Solar2Fuel concept). Additionally, the Solar2Fuel concept is compared to two other concepts: first, conventional power generation without CO_2 capture and conventional methanol production by natural gas reforming (reference concept); second, power generation with CO_2 capture and storage as well as conventional methanol production (CCS concept). Different options for CO_2 capture, MEA-scrubbing and membrane based separation, are investigated. Life cycle assessment (LCA) method is an appropriate tool to determine the overall ecological effects of the process chains of the concepts. Thereby, two functional units are used to analyse the concept (1 kWh electricity and 605 g methanol produced in a photocatalytic and conventional way).
Results in terms of environmental impacts are discussed in detail. Even though ecological impacts differ for the different CO_2 capture options, all results show that Solar2Fuel reduces CO2 emissions and therefore, the global warming potential in comparison to the other concepts. Furthermore, the primary energy demand and the acidification potential are reduced by the Solar2Fuel concept. With respect to the eutrophication potential no carbon capture but the reference concept is recommended. Regarding to the human toxicity potential Solar2Fuel concept can reduce emissions if membranes are used to capture CO_2. In contrast, the CCS concept can only reduce greenhouse gas emissions in comparison to the reference concept. All other environmental impacts increase by the CCS concept, with exception of the acidification potential of the MEA-scrubbing option in comparison to the reference concept.

MO 113

Life cycle risk assessment (LCRA): description of this methodological proposal and a case of study

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The life cycle of a product is generally characterized by the main following stages: Raw materials acquisition, Manufacturing, processing and formulation, Distribution and transportation, Use, re-use, maintenance, Recycle and Waste management. Considering the life cycle thinking in a risk analysis approach requires the adjustment of the classic risk analysis methodology. In order to build up this new methodology called Life Cycle Risk Assessment (LCRA), we relied on the Life Cycle Assessment (LCA) methodology, which allows the assessment of the potential environmental impacts throughout the life cycle of a system. Once these adjustments made, this LCRA new methodology is explained and applied to two energy pathways for transportation sector: hydrogen (produced from the biomass) and gasoline pathways.
The life cycle thinking is not taken into account in the traditional method of risk analysis. To integrate this fundamental concept to the risk analysis methodology following the model of the LCA (Life Cycle Assessment) methodology (ISO 14 040, 14044 and the ILCD Handbook), we made some adjustments to the risk analysis methodology. Each of the LCA's four steps has its counterpart in terms of LCRA (Life Cycle Risk Assessment). The variations between these two methodologies reside on two key steps of the LCA: the inventory (step 2) and the assessment (step 3). The inventory collects data whose nature is different between the two tools. For LCA, collected data are matter and energy flows; these data are qualitative and quantitative ones. For LCRA, the data collected are only qualitative since it is an inventory of dangerous situations. The assessment step consists of three sub-steps: classification, characterization and valuation, and allows a conversion of inventory data into results of impact / risk levels. For LCA, the conversion of inventory data is performed by a calculation using characterization factor. For LCRA, this conversion is done qualitatively by rating and prioritizing risks. However, the goal of sub-step classification is the same in both tools because it links the inventory data and the impacts/risk to be assessed. Just like the flow identified by a LCA that can contribute to different categories of impacts, dangerous situations can cause different types of accidents.
Therefore, limitations and hypotheses should be established to make the LCRA methodology usable and relevant in view of the objectives and the applicability of the expected results.

MO 114

Adapting life cycle assessment for multi-criteria analysis of a complex system: case study of urban mobility

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Urban mobility is identified as one of the most CO_2 emitters in France: transport represents 34% of CO_2 emissions in France in 2006 (ADEME 2006), including 25% of urban trip emissions. Some previous studies compare transport modes (Finkbeiner & Al. 2006), or assess CO_2 emissions that are related to urban mobility on a real case

(INSEE 2011). But literature is lacking about multi-criteria analysis of urban mobility in the general case. In particular, Life Cycle Assessment has not been largely used to qualify urban mobility impacts despite its possibility to evaluate the environmental impact (ISO14040, 2006).
Nevertheless, the complexity of the system "urban mobility"is a first difficulty to the evaluation, especially concerning the definition of goal and scope. The main topic of this poster is to find out a way to complete and adapt LCA in order to enable the evaluation of a complex system under the case study of urban mobility. We propose an approach based on the System Analysis Design Technique (SADT) that allows a clear and complete definition of the "urban mobility"system. Then the possibility to include more societal indicators beyond the environmental ones (such as noise, satisfaction of consumers, time travel, costs etc) will be studied. The final aim is to provide a configurable dynamic system to evaluate different scenarios of urban mobility.
The first results consist of a complete definition of the system that is based on a segmentation of urban mobility into sub-systems that constitute the "goal and objectives"step in LCA. This decomposition prepares to the next step of LCA, in which modal splits will be aggregated with elementary assessments of modes to obtain a multi-criteria analysis for several scenarios.
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MO 115
LCA of land-based freight transportation: including accidents in LCIA
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In this paper we performed an LCA of 12 land-based freight transport chains starting and/or ending in Switzerland. In the impact assessment, the ReCiPe method was used, extended with a method for the assessment of accidents. For each transport chain, all realistic transport modes were assessed (road, rail, and intermodal). The number of damaged persons and severity of injury were retrieved from statistical data and accident protocols for each mode of transportation. In order to translate this information to the Human Health endpoint category of the ReCiPe method, the number of damaged persons were weighted with weight and duration of the according injury type. The results show that in rail transport damage from accidents was negligible (<1% of the total human-health impact), while in road transport this share was between 20% and 36% of the total damage to human health. Since accident data on background processes was missing, the analysis could only be performed for the operation phase of the vehicles. Nevertheless, the relevancy of accident data in traffic operations could clearly be demonstrated for road transport indicating that accidents should be routinely considered in LCA studies in order not to miss impacts of high relevance.

Please see extended abstract for detailed information.

MO 116
Trends in transport-related human health impacts from life-cycle emissions and road accidents in Europe
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The analysis combined human health impacts generated from life cycle assessment with those generated from accident statistics. The aims were to compare the European trends in road safety with those of vehicle efficiency and emissions, and this in the context of the uncertainty surrounding the determination of emissions-related impacts. From an LCA perspective, the use of road vehicles causes emissions from the up and down-stream stages of the vehicle and vehicle fuel life-cycles as well as during use, and by applying conventional LCIA methodologies it is possible to achieve an impression of potential human health impacts quantified using the DALY (Disability adjusted life years). As a very different form of human health impact, the occurrence of road traffic accidents follows clear trends such that the consequences are an unfortunate aspect of motorized road use. Road accidents are accurately recorded and there is a large and readily available body of official statistics. The trends in both emissions and road accidents are, however, showing clear declines as vehicle engines become cleaner and road and vehicle safety increases, even as the overall number of registered vehicles and passenger kilometers in Europe continues to rise. For a calculation of DALY one requires not only years of life lost (YLL) but also years of life spent suffering disability (YLD) - the latter being appreciably more difficult to quantify with regard to the consequences of both emissions and accidents. Results of this initial study show not only similar orders of magnitude for impacts related to emissions and accidents but that, depending on the perspective applied to the characterisation of emissions-related impact factors and the current trends for both impact types, the impacts of accidents could still be higher.

MO 117
LCA of age-related environmental impact for biogenic hydraulic fluids
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Biogenic hydraulic fluids, based on synthetic esters, have an excellent environmental profile in the unused state, so that they are typically classified as 'not hazardous to water'. During storage at room temperature and tribological application, occurring chemical and toxicological changes take no account in the classification of lubricating oils until now. The ageing and oxidation stability gets increasing importance, since it determines the service life of lubricants in tribological systems in addition to the storage time. With an increased use of biogenic hydraulic fluids in environmentally sensitive areas, thus the need for an appropriate monitoring and assessment approach as part of a Life Cycle Assessment (LCA).
A lubricating oil mixture, based on high oleic sunflower oil, was monitored in an adapted life cycle for biogenic hydraulic fluids. For the detection of ecotoxicological effects, water soluble fractions (WSF) of oil samples with a real effect concentration of 100 g/L were prepared. Ecotoxicological testing was performed in standardised bioassays using 24- and 96-well microplates for algae and bacterial growth inhibition tests. Biodegradability was determined with the optimised test system "O_2/CO_2-Headspace Test".
After tribological application in an ageing test bench (48-192 h) there was only an increasing toxicity for the algae growth inhibition test as a function of time in contrast to the unused fluid with EL_{50}-values ranged from 80 % to 5 % (192 h). The ecotoxicity of hydraulic fluids increased depending on storage conditions. Storage at room temperature accelerates this process compared to 4°C. Compared to ecotoxicological behaviour by ageing during storage and use, a readily biodegradability within 28 days (≥ 70 %) was determined as it is demanded for the environmental label "Blue Angel"for biogenic hydraulic fluids.
Due to the quantification of metal content with ICP-MS in used hydraulic fluids and resultant WSF as well as the determination of the aqueos available metal content, there is a better interpretation and distinction of age-related aquatic ecotoxicity. The additional characterisation of conditional-use changes in ecological characteristics allows a comprehensive assessment and is still largely unknown, but an important aspect in terms of LCA for biogenic hydraulic fluids. This methodological approach thus allows the feedback of the desired product properties on the production method.

MO 118
Hydrotreated vegetable oil production in Spain: compliance with Directive 2009/28/EC in terms of GHG emissions savings
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Oil hydrotreating units in refineries are aimed at reducing the sulphur content of mineral fuels in order to get compliance with standard specifications. Moreover, this process is one of the best available technologies to obtain biofuels from vegetable oil at present. This study presents the GHG emissions of the biofuel HVO (Hydrotreated Vegetable Oil) obtained from vegetable oil by means of co-processing with conventional fossil fuel in hydrotreating facilities of two crude-oil refineries, using the LCA methodology. Results were compared with a mixture (in the same shares) of FAME (Fatty Acid Methyl Ester), a biofuel obtained by means of transesterification of vegetable oil, and mineral diesel. Results highlight that the HVO mixed with mineral diesel has at least the same environmental performance compared to a mixture of FAME and mineral diesel. GHG emissions savings compared to standard diesel from Renevable Energy European Directive 2009/28/Ec are exposed. In addition, sensitivity analysis have been conducted in order to assess the influence in results of different data sources and different allocation processes that LCA standards suggest, showing the most relevant hot-spots that influence the improvement of previous results.

MO 119
Life cycle assessment of chitosan-based films
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Conventional plastic films used nowadays for food packaging are based on non-renewable sources, non-biodegradable and impact heavily on the environment. For all these reasons, a new biodegradable packaging material based on renewable raw materials has been developed. Chitosan is the second most abundant polysaccharide found in nature and has non-toxic, biodegradable, and antimicrobial characteristics, which are of great interest for food packaging purposes. Chitosan is mainly manufactured from crustaceans due to the large amount of its skeleton available as a by-product of food processing. In this context, chitosan is an interesting film forming material.
A comparative life cycle assessment between two different food packaging systems has been carried out: a commercial food packaging film based on polypropylene (PP) and a new biodegradable chitosan-based film manufactured in our labs. The environmental load of chitosan-based films in different stages of its life cycle has been studied and compared with the one of conventional PP films used as food cover.
The functional unit considered in this study is 1 m2 of similar thickness packaging film. The studied system includes three main stages: material obtaining, film manufacture, and end of life. The data relating to PP packaging films were obtained from Ecoinvent v2.0 database, developed. The life cycle inventory for chitosan powder from crustacean shell was taken from literature and film manufacture data was measured directly by our research group in the lab. The EcoIndicator 99 method was selected for comparison of the films.
Obtained results showed that PP film has a higher impact than chitosan-based film in carcinogens and fossil fuels impact categories. The environmental burden associated to carcinogens is mainly due to the end of life stage, while the impact related to fossil fuels is owing to the extraction of PP. On the contrary, the categories in which chitosan-based film has a higher environmental load are respiratory inorganics, land use and minerals. Environmental load associated to respiratory inorganics is mostly related to the

acetic acid used in film manufacture and, in a more significant way, to the hydrochloric acid used in the raw materials extraction, which is also responsible for the impact in minerals category in the raw materials extraction stage. In addition, the main responsible for land use is the glycerine used in the film manufacture stage considered as a by product from biodiesel.

MO 120
Environmental indicators, as a result of the Life Cycle Assessment application for the Mexican corrugated cardboard industry
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Considering the present situation in Mexico, the environmental protection and the responsible use of the available resources are current needs. The involvement of each of the industries in the country is essential to achieve tangible results for the environmental welfare.
The Life Cycle Assessment (LCA) is used for this study with the objective of making a comparison between the use of virgin, and the use of recycled raw materials in the production of corrugated cardboard, under Mexican conditions. The contribution of applying LCA works to identify different environmental impacts from the individual processes of the complete system.
The identification of the environmental impacts runs in order to consider specific aspects, which would focus on the sustainability of the enterprises involved in the corrugated cardboard manufacturing industry. The aspects identified could be properly implemented in the future as a functional part of an environmental policy proposal.
The results showed that the system of the recycled corrugated cardboard production impacts less in every environmental impact category analyzed, than the virgin corrugated cardboard production. However, in Mexico, it is a system that can be optimized through specific activities; especially in the manufacturing and transportation processes, where the greater environmental impacts were located.

MO 121
GHG emissions comparison of tissue paper from virgin pulp vs. recycled waste paper
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Pulp and paper manufacturing industry is the fourth largest greenhouse gases (GHG) emitter and is responsible for around 9% of the total global CO_2 emissions from manufacturing sectors. The increasing trend of paper consumption is one of the principal drivers behind the emissions from the sector. Therefore, policy measures which ensure not only the reduction in consumption of paper but also the increasing use of recycled waste paper, the implementation of cleaner production practices and the use of fibres from sustainable sources are of main importance. The aim of this work is to compare the environmental implications of tissue paper produced from virgin pulp (VP) vs. recycled waste paper (RWP). By doing so, this work informs decision-makers both at company or national levels on the main driving forces behind emissions generation and suggests necessary actions to decrease pollution. The main questions which this work addresses are: how the choice of raw materials for the VP and RWP processes influences the life cycle GHG emissions of tissue paper production? what are the main drivers behind the se emissions? which is the share in emissions generation of the direct material and energy requirements or of transportation? All these aspects are analysed by considering all the stages involved in the life cycle of tissue paper production and identifying the most relevant processes that have significant contribution to the global GHG emissions of the product. Our results show that the energy demand in the form of electricity and steam is relatively higher in the case of RWP process than VP process, if only the manufacturing stages are considered. However, different picture comes out when the comparison is based on the entire life cycle of the product. The GHG emissions from the VP process are about 24% higher than the RWP process. This implies a saving of 424 g eq CO_2 for each kg of tissue paper produced from RWP instead from VP. GHG emissions from pulping process alone, 470 g eq CO_2 per kg of tissue paper, were about 3 times higher than emissions from waste paper collection and transportation. According to our results, replacing recycled waste paper for virgin pulp has environmental benefits.

EP02P - Endocrine disrupting chemicals: recent developments

MO 122
Combination of Planar Chromatography with in vitro bioassays as a tool for effect directed analysis
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The identification of environmental contamination with a (specific) biological activity is demanding due to the vast number of compounds which are released in the environment by humans. In recent years various strategies and methods were developed for an effect directed analysis which in general combine separation methods like LC or HPLC with biological assays and a subsequent chemical analysis of fractions which are biologically active.
Beside the complexity of chemical mixtures in the environment, the often low concentrations of contaminants are a further challenge, especially in case of anthropogenic micropollutants with specific modes of action like drugs or endocrine disruptors. In order to overcome these difficulties, environmental samples are usually concentrated by solid phase extractions (SPE). However, potential active compounds which are not bound to the matrix of the solid phase are not concentrated and so the SPE might already result in a separation of the sample. They might be even lost if the flow-through of the SPE is not further characterized.
An alternative to the method described above is the use of planar chromatography (HPTLC) in combination with bioassays. Samples can be easily concentrated on a thin layer plate by multiple sample application and/or a focusing step if a multi development method is used for the chromatography. The challenge of this strategy is to perform bioassays for the detection of specific effects directly on the surface of the thin layer plate. Therefore, these bioassays have to be adapted for this new application.
The combination of thin layer chromatography with the luminous bacteria test for the detection of acute toxic effects is already well described and frequently used. In contrast, studies showing the coupling of HPTLC with specific bioassays like the Yeast Estrogen Screen (YES) are scarce. The objective of the presented work is to develop and optimize techniques for the combination of HPTLC with various specific bioassays and to test the hypothesis that such an approach is a useful tool for the effect directed analysis of environmental samples.

MO 123
Development of a multi-component detection method for with UPLC-tQ-MS/MS to identify steroid hormones in CALUX positive surface water samples
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Surface waters, such as the rivers Rhine and Meuse, are important sources for the drinking water supply in the Netherlands. Dutch drinking water companies therefore intensively investigate their water sources for the presence of emerging contaminants and their fate during treatment processes. One of the classes of concern are compounds with endocrine disrupting, e.g. estrogenic, activity. Nowadays, natural and synthetic steroidal estrogens are known as the primary causative agents of estrogenic activity in the aquatic environment. With the development of new bioassays, it has become possible to investigate also the activity of other classes of steroid hormones and compounds with comparable or antagonistic activities. Many hormone-like compounds are excreted naturally or are used as pharmaceuticals and might thus enter the environment via similar routes as estrogens. Indeed, using CALUX bioassays for progestagenic, androgenic, estrogenic and glucocorticoid receptor activation, the presence of especially glucocorticoid activity in Dutch surface waters and glucocorticoids in waste water was recently reported. Now that activity is found, methods are needed for the identification of the responsible compounds. Due to the low environmental concentrations, an analysis sensitivity is required that is currently only feasible by target analysis methods. We developed a highly sensitive multi-component analysis method for over 40 natural and synthetic steroid hormones in water, including estrogens, androgens, progestagens and glucocorticosteroids. The method uses Ultra Performance Liquid Chromatography separation followed by tandem Mass Spectrometry detection (UPLC-MS/MS). Due to the narrow bore (i.d. 2.1 mm) column packed with small C18 particles (size 1,7 µm), improved separation power and detection limits and reduced analysis times are achieved in comparison with conventional LC-MS. The method was applied to samples from Rhine and Meuse and results were compared with results from the CALUX analyses of hormone-like activity in samples from the same locations.

MO 124
Development of simultaneous analysis technique for phthalate di- and mono-esters using online-SPE and high speed mass spectrometer
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Simultaneous analysis technique for trace amount of phthalate di- and mono-esters was developed and applied to aqueous samples. Phthalate esters are used as plasticizers and often reported to have endocrine disrupting activities. When phthalate di-esters are taken up into the body, they are metabolized into mono-esters and excreted to urine. Since both di- and mono-phthalates are likely to exist as mixture in the environmental water and wastewater, it is important to develop a simultaneous quantification method for both forms. Recently some researchers reported the advantage of using on-line SPE system couple with LC-MS/MS determination which gives easy and high throughput analysis. This technique also provides greater reproducibility of pretreatment processes. To achieve high throughput analytical methods, not only the on-line SPE system but also high speed mass spectrometer is required. Phthalate esters have various homologues with different alkyl side chains. Positive ionisation is more suitable for phthalate di-esters while negative ionization for mono-esters. The mass spectrometer used in this study were capable of high speed MRM (500 ch/s) and polarity switching (15 ms). This presentation reports simultaneous analysis of the phthalate di- and mono-esters using online-SPE system and simultaneous positive/negative electro-spray ionization.

MO 125
Synthesis and identification of novel metabolites of polybrominated diphenyl ethers in human blood
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Hydroxylated polybrominated diphenyl ethers (OH-PDBEs) are exogenous, bioactive compounds that originate, to a large extent, from antropogenic activities, although they are also naturally produced in the environment. In the present study nine new authentic OH-PBDE reference standards and their corresponding methyl ether derivatives (MeO-PBDEs) were synthesised and characterised by NMR spectroscopy and mass spectrometry. Seven of the prepared authentic reference standards were thereafter identified in a pooled human blood sample. The identified OH-PBDEs were 3-hydroxy-2,2',4,4',6-pentabromodiphenyl ether, 3'-hydroxy-2,2',4,4',6-pentabromodiphenyl ether, 3-hydroxy-2,2',4,4',5-pentabromodiphenyl ether, 3-hydroxy-2,2',4,4',5,6'-hexabromodiphenyl ether, 3'-hydroxy-2,2',4,4',5,6'-hexabromodiphenyl ether, 3-hydroxy-2,2',4,4',5,5'-hexabromodiphenyl ether and 4-hydroxy-2,2',3,4',5,5',6-heptabromodiphenyl ether. An additional seven OH-PBDEs were identified in the pooled human blood sample, of which one OH-PBDE, 4'-hydroxy-2,2',4,5,5'-pentabromodiphenyl ether, has not been identified in human blood before. The identification was performed using gas chromatography-mass spectrometry (GC-MS) recording the bromine ions m/z 79, 81. The identification was supported by the peaks relative retention times (RRTs) compared to authentic references on two GC columns of different polaritys for the hexa-, and heptabrominated OH-PBDEs, and three different GC columns for the pentabrominated OH-PBDEs. The OH-PBDE congeners most likely originate from human metabolism of the flame retardant polybrominated diphenyl ethers due to the relatively high concentrations of PBDEs in the same human blood sample and the strong metabolic relationship between OH-PBDEs and their parent PBDEs.

MO 126

Isolation and identification of ligands for the goldfish testicular androgen receptor in chemical recovery condensates from a Canadian bleached kraft pulp and paper mill

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This study builds on a series of investigations characterizing substances in kraft mill chemical recovery condensates that depress sex steroids in fish. Here, incubations of goldfish testis androgen receptors (AR) with condensate extracts were used to investigate the potential role of androgens in hormone depressions. Condensates contained variable levels of AR ligands, with the highest amounts in nonpolar extracts of filtered solids prior to solid phase extraction (SPE). High pressure liquid chromatography (HPLC) fractionation recovered the majority of activity in one fraction, with ligands detected in three additional fractions. Gas chromatography mass spectrometry analysis of the most active fraction confirmed the two most abundant components as the diterpenes manool and geranyl linalool. Manool exhibited a relative affinity for the AR that was 300 fold less than testosterone and accounted for 26% of total filtered solids activity. Geranyl linalool exhibited no affinity for the AR. Three additional diterpenoid families were tentatively identified as principal components of the three other androgenic HPLC fractions. Compared to condensates, final effluent had 3000 fold less androgenic activity, with <1% attributable to manool. Putative androgens previously associated with mill effluents (androstenedione and androstadienedione) and progesterone were not detected; however, additional condensate diterpenes suspected as androgens were identified in final effluent. This study is the first to confirm nonsteroidal cyclic diterpenes as androgenic at pulp mills. A major in-mill source of these substances was identified, and the role of androgens in mill effluents affecting fish reproduction was reinforced.

MO 127

Thyroid hormone disruption in effect-directed analysis - An endpoint of growing concern

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Thyroid hormones (THs) play an important role in the maintenance of a normal physiological state. Chemicals in the environment that interfere with the ability of the thyroid hormone system to function normally could have devastating effects on individuals, as well as on whole populations. Serum transport proteins are important in regulating total hormone levels by influencing the transport capacity of the TH, which are lipophilic compounds poorly soluble in the blood. TDCs can bind to transport protein and hence replace the natural THs; hindering the THs to reach their target organs.
In Effect-Directed Analysis (EDA), various bioassays have been implemented that have an endpoint related to endocrine disruption. We have used the radioligand TTR-binding assay to direct our fractionation for the identification of unknown TDCs in environmental samples. In addition, to assess what classes of environmental toxicants are capable of interfering with the TH system, an inventory of the literature describing compounds with reported potency to bind to the TH transport protein TTR was made. Compounds that are known to influence the thyroid system (e.g. hydroxylated PBDEs and PCBs, triclosan, DDE, TBBPA) all have structural similarities with the natural hormone Thyroxin (T4), i.e. an aromatic ring with a hydroxyl-group and adjacent halogens. But more recently, also polyfluoroalkyl substances were shown to have moderate TTR binding potencies. The presence of functional groups together with the length of the fluorinated carbon chain was a crucial factor for binding to the TTR binding site. This shows that more compound groups than the phenolic aromatic halogens are capable of disrupting the thyroid hormone system.
Using GC-MS, 43 compounds were tentatively identified in the sediment and 57 compounds was tentatively identified with LC-HRMS. In total, 25 of these compounds were purchased and tested in the TTR-assay: only 4 compounds showed a response. For the sediment fractions, only a very small part of the response could be explained by the presence of the tested compounds. In order to enhance the identification of these unknown compounds that can bind to TTR and hence may be disruptors of the thyroid hormone system, it is necessary to develop identification strategies using e.g. high resolution mass spectrometry and compound lists and mass spectrometric libraries need to be further developed.

MO 128

Estrogenicity of 75 European waste water effluents evaluated by in vitro assay

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Various natural and synthetic contaminants present in urban waste waters have been shown to posses estrogenic activity, and many questions related to the risks of these compounds are not fully resolved. Under environmental conditions, steroidal hormones appear to be primarily responsible for adverse effects observed in fish downstream of waste water treatment plants (WWTPs)However, instrumental analyses of steroidal estrogens often fail in detection of their actual concentrations in complex environmental matrices such as waste water effluents. In the present study MVLN in vitro assay was used to evaluate estrogenicity of 75 European waste water effluents. The samples originated from the FATE-SEES 2010 pan-European monitoring campaign coordinated by the European Commission's Joint Research Centre (JRC) in Ispra, Italy. Estrogenic activity was expressed as 17β-estradiol equivalents (EEq). Twenty seven sample extracts showed significant estrogenic activity higher than the detection limit >0.5 ng/L EEq with values ranging 0.53 to 17.9 ng/L EEq. The highest activities have been detected in WWTPs at some of the major European capital cities indicating the importance of this contamination source. Our study provides some of the first EU-wide snapshot data on the estrogenicity of WWTP effluents, and demonstrates suitability of in vitro bioassays as effect-based monitoring tools.

MO 129

Assessing the endocrine activity of sediment samples from Laguna Lake, Philippines, using the LYES and H295R assays

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Due to the increasing use of diverse chemicals by modern society, nearly every living space is affected by numerous known and unknown chemicals of anthropogenic origin. Since the early 1990s there is increasing concern about the exposure to chemicals that have the potential to interact with the endocrine system and associated physiological functions in human and wildlife. The present study was conducted to further investigate the level of contamination of sediment samples from Laguna Lake. The said lake is the second largest freshwater lake in Southeast Asia and the largest lake in the Philippines. It is also a member of the Living Lakes Network since 2001. Based on preliminary results, the present study selected sediment samples of two different sites for fractionation and effect-directed analysis: Central Bay (S5) and East Bay (S8). While the watershed around the Central Bay is urbanized and industrialized, that around East Bay is basically residential and agricultural area. In this study the LYES-Assay (Yeast estrogenic screen assay assisted by enzymatic digestion with Lyticase) was performed to screen for estrogenic active fractions in sediment samples from Laguna Lake. As a further investigation the crude extracts of five main sites have been tested in the H295R-Assay for their potential to disrupt steroidogenesis pathways. The sediment samples have been extracted by using an accelerated solvent extraction method (ASE 300, Dionex Corp., Sunnyvale, CA, USA). The fractionation of Central Bay and East Bay extracts was conducted using an automated multistep fractionation method developed by Lübcke van Varel et. al. (2008). In the sediment samples from East Bay four fractions showed a significant endocrine effectiveness at the one fold concentration (fraction 11, 15, 16, 18). The estrogenic activity ranged from 8.43 ± 4.37 ng/L at fraction 18 to 10.79 ± 5.28 ng/L at fraction 15. Fraction 16 also revealed a significant endocrine effectiveness at the ½ fold concentration of 12.59 ± 9.91 ng/L. Only one fraction indicated a significant endocrine potential from sediment samples of Central Bay. Indeed, fraction 18 revealed significant endocrine effectiveness at the 1/8 fold concentration of 8.80 ± 2.29 ng/L up to 27.32 ± 18.39 ng/L at the one fold concentration. In the H295R-Assay all crude extracts showed an increase of the 17β-estradiol production. It ranged from 589.62 ± 116.31 pg/ml E2 at Central Bay (S5) to 1833.57 ± 146.24 pg/ml E2 at South Bay (S10).

MO 130

Effects of 4-nonylphenol and/or diisononylphthalate on THP-1 cells: impact of endocrine disruptors on human immune system parameters

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The aim of the present work was to investigate the link of two endocrine disruptors compounds (EDCs) and the human immune response through a study of their effects on the THP-1 human cell line which was used as a model for macrophages. We used two EDCs, diisononylphthalate (DiP) and 4-n-nonylphenol (NP) alone or in combination in order to evaluate the effects of these compounds on several parameters of the immune response: cytokine secretion, phagocytosis and the putative implication of the estrogen receptors by studying the level of MAPK activation. NP and DiP strongly reduced phagocytosis and modify cytokine secretions. Indeed, THP-1 cell exposures (i) to 5 and 10 µM of combination of NP and DiP induced an IL-8 level in the medium respectively 28.9 and 45% higher than level obtain for control (untreated cells), (ii) to combination

of NP and DiP at 10 µM induced an increase of IL-1 beta level in comparison to the control level, (iii) to combination of NP and DiP induced an increase of TNF-alpha level whatever the concentration of EDCs tested (between 0 and 10 µM). Last, THP-1 cell exposure to NP, DiP alone or in combination (2 µM for each condition) induced a decrease of ERK1/2 phosphorylation in comparison to ERK1/2 phosphorylation level of control. Moreover, THP-1 cell treatments by ICI-182780 (an estrogen receptor antagonist) supressed the EDCs effects on ERK1/2 phosphorylation level which indicates an estrogen receptor-dependent pathway.
These results suggest that EDCs have the ability to alter the human immune function, maybe by interfering with endocrine balance.

MO 131
Rapid determination of bisphenol A in water by amperometry using a tyrosinase biosensor
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Recently, Bisphenol A (BPA) has received considerable attention because of its interfering the endocrine system of wildlife and human, increasing cancer rate, etc. In this work, we prepared a novel electrochemical biosensor for the rapid determination of BPA.

A 10µL aliquot of 1.0mg/mL the treated mutiwall carbon nanotubes (MWNTs) solution was cast on the surface of a glassy carbon electrode (GCE), dried in air. Gold nanoparticles were electrodeposited onto the MWNTs modified electrode by amperometry at 1.5V for 5min from a fresh colloidal gold solution which was prepared with 0.01% HAuCl4. The modified electrode was denoted as Au/MWNTs/GCE. A 7µL aliquot enzyme solution containing tyrosinase (Tyr) and Silk fibroin was then dropped on the surface of the Au/MWNTs/GCE, allowed to dryness at room temperature. This enzyme activity was approximately equal to 40U on each electrode surface. All electrochemical measurements were performed with CHI650c electrochemical analyzer. A bare or film modified GCE with a diameter of 3 mm was used as working electrode, a platinum wire as auxiliary electrode and a saturated calomel electrode (SCE) as the reference, respectively.
The SEM image of the Au/MWNTs/GCE showed that the diameter of the Au nanoparticles dispersed on the MWNTs was about 10 nm. In the presence of molecular oxygen, the tyrosinase can catalyse the oxidation of BPA to o-quinones. The experimental results of cyclic voltammetry showed that the reduction peak current increased with the BPA added. MWCNTs and gold nanoparticles possessed excellent synergistic electrocatalytic effect to enhance the electron transfer rate. The amperometric cathodic current is proportional to BPA concentration in 0.1M pH 7.5 phosphate buffer solution over the range from 0.2µM to 8.0µM with a correlation coefficient of 0.9991 and a detection limit of 0.1µM. The method was applied to the determination of BPA in real water samples. The experimental results showed the biosensor possessed high sensitivity, good selectivity and stability towards the determination of BPA.
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MO 132
Evaluating endocrine activity in plant leaf extracts: temperature and solvent choice influence androgenic, oestrogenic and progestogenic activity in vitro and in vivo
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The goal of this research is to characterize the in vitro and in vivo activities of plant-derived endocrine active compounds (EACs) and to evaluate potential effects of relevance to fish reproductive health. In contrast to mammalian species, there is a scarcity of knowledge on the importance of plant-derived EACs for fish and aquatic life. A scientifically reliable assessment of the potential impacts of synthetic EACs on fish health therefore depends on a holistic assessment of cumulative aquatic exposures to EACs of specific modes of action pertinent to fish reproduction (especially androgens, oestrogens and progestins). Currently, leaf material was collected from three woodland and marsh sites in south west England and processed for screening using a battery of (anti)estrogenic, (anti)androgenic and (anti)gestagenic in vitro screens (the YAS, YES and YPS assays, respectively). Key factors that have been addressed during the first phase of work are the impact of temperature and solvent on the extraction of dissolved organic carbon (DOC) and consequent responses in the YAS, YES and YPS assays (as both agonism and antagonism). For each plant species sampled, beech (Fagus sylvatica), oak (Quercus robur) and reed (Phragmites australis), ca. 30L of dried leaves were collected from April to June 2011. Leaves were air dried (7d) then stored @ -80°C before homogenization in water for 24 h at 20, 15 or 4°C. The aqueous extracts (approx 2L) were stored at -80°C and subsamples used to measure DOC. Aqueous extracts (10 µl volumes) were directly screened in the YAS, YES and YPS assays. In addition, aqueous extract subsamples (10 ml) were concentrated by solid phase extraction (SPE) onto a Sep-Pak C18 cartridge which was then eluted with methanol. The samples were dried under vacuum before being resuspended in ethanol. The concentrated extracts were then also screened in the YAS, YES and YPS assays. Extraction temperature had a marked proportionate effect on aqueous DOC values. For the reed aqueous extracts, there was a DOC-related response in the YES assay. For the beech and oak extracts, there were variable responses in the various yeast assays. The information generated in this study will be used to support further characterisation of EACs in plant leaf material using a range of in vitro screens and in vivo fish test protocols. This work is funded by the CEFIC Long-range Research Initiative (RfP reference EMSG55).

MO 133
Utilizing a functional, sensitive, and specific cell-based assay for screening potential endocrine active chemicals
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Endocrine active chemicals are thought to produce endocrine disruptive effects in humans and wildlife by interfering with steroid hormone signaling. Environmental contaminants and industrial pollutants that interact with estrogen and androgen receptors can profoundly affect normal development and hormonal homeostasis and are suspected in numerous health and reproductive problems in both humans and wildlife. Regulatory mandates requiring endocrine disruption risk assessment for consumer products present major obstacles to current testing procedures which are expensive, time consuming, and require large numbers of animals. These obstacles can be overcome by automating procedures to assess endocrine activity in vitro using high content cell-based assays as a pre-screen and such in vitro screens for potential endocrine active chemicals (EACs) reduce animal testing by categorizing and prioritizing chemicals based on their effect on endocrine receptor activity.
Two cell-based assays were used to efficiently test chemicals for their ability to activate GFP-tagged steroid receptors estrogen receptor alpha (ERα) and androgen receptor (AR). These biosensors form nuclear foci in response to stimulation that can be easily quantified by automated fluorescence imaging (high-content). Additional outputs for individual cells are simultaneously measured resulting in direct assessment of compound toxicity and comparison to positive controls, thus providing insight into the dynamics of receptor activation while simultaneously monitoring cell cycle perturbations and toxicity. Compared to currently validated in vitro endocrine disruption assays, these cell-based functional assays resulted in higher specificity and sensitivity (>80%) against a panel of compounds that included pesticides, phytoestrogens, and plasticizers. Bisphenol A was detected by the ERα assay at ~66 ppb, which is more sensitive than the current allowable intake limits from several regulatory agencies. The assays were developed following EPA and ICCVAM guidelines for endocrine disruption assays and provide functional in vitro determination of receptor activity, resulting in a more thorough assessment of the potential for in vivo endocrine disruption.

MO 134
Development of an in vitro model for screening EDCs and deciphering the specific target sites along the HPG axis
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Currently, the vast majority of studies on endocrine disrupting chemicals are based on *in vivo* approaches. The intrinsic complexity of the neuroendocrine and endocrine systems in *in vivo* system often makes it difficult to decipher the target sites and action mechanisms of endocrine disrupting chemicals (EDCs) in specific organs. As such, studies using *in vitro* systems are required to provide information complementary to *in vivo* studies, and to provide important insights into the action mechanisms of EDCs in specific organs. We have successfully developed primary cell cultures (pituitary, ovarian follicular and testicular cells) in the marine medaka (*Oryzias melastigma*), a universal model for marine environmental study. Using these *in vitro* systems, we have performed a series of experiments to elucidate the effects of different EDCs at different levels of the medaka HPG axis, particularly on steroidogenesis in the gonads. To validate these systems, individual cell types were challenged with environmentally relevant concentrations of common EDCs including polybrominated diphenyl ethers (PBDE), 4-nonylphenol (NP) as well as hypoxia. The expression levels of various steroidogenic genes (including *cyp19a*, *cyp11a*, *3bhsd*, *20bhsd*, *star*, etc.) were analyzed by quantitative real-time RT-PCR. Among the steroidogenic genes studied, aromatase (*cyp19a*) was responsive to almost all treatments, suggesting that it is a major target site for endocrine disruption. The results obtained from these *in vitro* studies were compared to those obtained from *in vivo* exposure of whole fish as well as from H295R, a human cell line. Although different systems did not generate identical expression responses to the same chemical exposure on all parameters, the results were largely comparable. Our results suggest that medaka primary cell cultures not only serve as a useful tool for screening EDCs, but also provide a platform for deciphering the specific target site of EDCs along the HPG axis and their action mechanisms.

MO 135
TTR binding of metabolite extracts from biological matrices: identification, quantification and TTR binding potency of co-extractants from microsomal extracts
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PCB and BDE metabolites are retained in tissues, particularly in blood, and are considered to be the main cause of several observed POP effects. Thus, transport protein binding of metabolites coming from plasma and/or from biologically activated extracts becomes of paramount importance within risk assessment. However, efforts to apply TTR binding methods to biological matrices have encountered insurmountable technical problems or required copious procedures to succeed. Free fatty acids interact with transport proteins like transthyretin (TTR), and with the hormone thyroxin (T4) interfering with the competitive binding and ultimately preventing the analysis. However, it is not exactly known which are the co-extracted compounds from various biological matrices that present a problem for the competitive binding analysis. We aimed to identify and quantify the co-extractants from a biological matrix and their potency to interfere with the TTR competitive binding analysis to understand the problem dimension and enable its future solution. Incubations of rat liver S9 fraction were extracted according to published methods and co-extractants were identified and quantified through GC/MS analysis after sylilation. Saturated fatty acids (SFA), non-saturated fatty acids (NSFA) and cholesterol were identified as the prevalent co-extractants. At current dilution factors, co-extractant concentrations ranged from 8-26 µM of SFA, 2-5 µM NSFA and 0.2-1.4 µM of cholesterol. The potency of identified co-extractants was determined in a 96-well plate using the competitive displacement of the ANSA fluorophore (Ka = 1.5 µM) from TTR . Although less sensitive (T4 EC50 = 300 nM), this method is high

throughput and it does not require radioactive ligand or expensive equipment . SFAs partially displaced the fluorophore from TTR with an average EC50 of 1.6 µM, while NSFA completely displaced it with an average EC50 of 1.0 µM. Given the typical co-extractant concentrations, the fatty acids in the extract are the most likely cause of the interference. Due to their physicochemical similarities, complete separation of POP metabolites from fat has been only possible through derivatization and acid clean-up, which will render the metabolites unsuitable for biological testing. As further dilution will weaken the detection limit, a method to selectively remove the fatty acids is currently under validation.

MO 136

Tetrabromobisphenol-A disrupts thyroid hormone receptor alpha function in vitro: use of fluorescence polarization to assay corepressor and coactivator peptide binding

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Thyroid hormone receptors (TRs) recruit corepressor or coactivator factors to the promoters of target genes to regulate their transcription. Corepressors such as nuclear hormone receptor corepressor (NCoR) are recruited by unliganded TRs, whereas coactivators such as steroid receptor coactivator-1 (SRC1/2) are recruited when triiodothyronine (T3) is bound to TRs. These coregulator proteins interact with the ligand binding domain (LBD) of TRs via short, conserved peptide sequences that can be used to probe the conformational changes induced in TR LBD by TR ligands. Recombinant LBD of the human TR 1 isoform (hTR 1 LBD) was produced as a fusion with glutathione S-transferase, and used to develop assays based on fluorescence polarization to quantify the binding of either NCoR- or SRC1/2-derived fluorescent peptides to the hTR 1 LBD. Under predefined conditions, T3 induced a dose-dependent decrease in NCoR peptide binding, and a reciprocal dose-dependent increase in SRC2 peptide binding, in both cases at similar 50%-effective doses. The TR agonists triiodothyroacetic acid and thyroxine were also effective in preventing NCoR peptide binding and increasing SRC2 peptide binding, whereas reverse-triiodothyronine was less efficient and the biologically inactive thyronine had no effect on either process. These experiments validate cell-free assays based on the use of binding of corepressor or coactivator peptide probes, as measured by fluorescence polarization, for investigating the conformational changes of TR 1 LBD induced by potentially TR-interfering compounds. Both these methods were used to elucidate the mechanism of the disrupting effects of tetrabromobisphenol-A (TBBPA) on the hTR 1 LBD conformation related to the transcriptional activity of the receptor. TBBPA is a flame retardant that is released into the environment, and is a suspected disrupter of thyroid homeostasis. The present results indicate that TBBPA did indeed interfere with the ability of the hTR 1 LBD to bind both NCoR and SRC2. TBBPA behaved similarly to T3 in promoting the release of NCoR from LBD, whereas it failed to promote LBD interactions with SRC2. However, it did reduce the T3-induced interactions between LBD and the coactivator peptide. This study therefore suggests that TBBPA in the micromolar range can affect the regulation of transcription by both the apo- and the holo-TR 1, with potential disruption of the expression of genes that are either up- or down-regulated by T3.

MO 137

The other endocrine activity: in vitro screening of sewage treatment plant effluents for retinoid, thyroid and vitamin D receptor agonists

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In the past, immense scientific and regulatory attention has been paid to environmental chemicals interfering with steroid receptors, especially to estrogenic and anti-androgenic compounds. Doubtlessly, focusing on androgens and estrogens is important since they are key players in reproduction and development. However, besides androgen and estrogen receptors there is a plethora of transcription factors controlled by other than steroid hormones. To elucidate potential effects mediated via non-steroidal pathways, environmental toxicology needs to widen the focus to effects mediated via other hormone receptors.
In this context, we employ Yeast Two Hybrid assays with thyroid receptor (TR), retinoid X receptor (RXR), vitamin D receptor (VDR), and retinoic acid receptor (RAR) in order to characterize the endocrine activity of 78 effluents sampled at 51 industrial and municipal sewage treatment plants (STP). To avoid the loss of active compounds, water samples were analyzed without further treatment, e.g. filtration or solid phase extraction (SPE).
STP effluents did not induce TR, RXR, or VDR activity. Compared to that, 54 of 78 effluents (69%) significantly activated RAR. This retinoid activity was very potent: Expressed relative to the endogenous ligand all-trans retinoic acid (ATRA), we detected a mean of 241 ng L-1 ATRA-EQ and a maximum of 2160 ng L-1 ATRA-EQ. Since other studies analyzed solid phase extracts of STP effluents and detected a much lower activity, we evaluated the suitability of several SPE methods to concentrate the RAR agonists. Since none of the procedures was able to extract significant levels of RAR activity we conclude that the causative chemicals are poorly extractable and thus might be missed when analyzing SPE extracts solely.
In a more general context, our data indicate that the investigated STPs are a source of chemicals that activate the retinoic acid receptor. Since the responsible chemicals are so-far unidentified, potential in vivo consequences remain to be evaluated. However, in the light of the known teratogenicity of some retinoids, an identification and further toxicological characterization of these 'emerging' chemicals is imperative.

MO 138

The endocrine disrupting effect of hypoxia on pituitary cells

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Hypoxia is an endocrine disruptor which can affect the synthesis and balance of sex hormones and thereby impairs reproduction of fish. However, the precise mechanisms of endocrine disruption remain unclear. Moreover, effects of hypoxia on reproduction in higher vertebrates such as mammals remain largely unknown. Gonadotropin releasing hormone (GnRH) is known to play a pivotal role in vertebrate reproduction. Previous studies have suggested that suppressed expression of GnRH and/or GnRH receptor (GnRHR) along the Hypothalamus-Pituitary-Gonad (HPG) axis could be an important mechanism contributing to reproductive impairments in hypoxic fish. Given that the HPG axis and genes controlling steroidogenesis as well as the sex hormones are highly conserved across vertebrate groups, the endocrine-disrupting effects of hypoxia found in fish may also occur in mammals including human. The aim of the present study is to determine whether hypoxia would affect the expression of GnRHR gene (one of the key genes along the HPG axis) in mammalian pituitary cells. A mouse pituitary cell line, LbetaT2, was used as an in vitro model to test the hypothesis that hypoxia can affect the expression of GnRHR in pituitary, thereby affecting reproduction in mammals. LbetaT2 cells were incubated for 24, 36, or 48 hours in a hypoxic chamber with 2% O2 and an identical set of cells were incubated under normoxic condition to serve as controls. The expression level of GnRHR mRNA was subsequently determined by SYBR Green-based real-time RT-PCR. Furthermore, the effect of hypoxia on transcriptional activity of GnRHR gene in the LbetaT2 pituitary cells was determined. A 1.2 kb fragment of mouse GnRHR promoter was cloned into pGL3-Basic vector and transfected into the LbetaT2 cells. The transfected cells were put into hypoxic chamber with 2% O2 and incubated for 24, 36, or 48 hours. The promoter activity determined from hypoxic cells was compared with that determined from normoxic cells. The effects of hypoxia on GnRHR gene expression and promoter activity in the LbetaT2 pituitary cells will be discussed in this presentation. Our current study represents the first important attempt to decipher the effects of hypoxia (an endocrine disruptor) on mammalian reproduction.

MO 139

Gammarus pulex responses to short-term exposure towards endocrine disruptors and pharmaceuticals in waste water

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Gammarus pulex is one of the most frequent and abundant freshwater amphipod in European streams, playing an important key-role in the aquatic food web and detritus cycling. Moreover, Gammarus pulex is sensitive towards pollution. Endocrine disruptors and pharmaceuticals are important chemcials in the effluent of urban waste water treatment plants. Traditional purification steps cannot completely remove these so-called micropollutants.
Gammarus pulex has been used in the fully automated real-time based Multispecies Freshwater Biomonitor[TRADEMARK] (MFB) to detect rapidly low concentrations of different micropollutants released in municipal waste water studying behavior (locomotion, ventilation) and survival. Moreover, the removal of the ecotoxicological potential in different treatment steps was recorded in short and long-term exposures.

MO 140

Do Bacillus thuringiensis israelensis products affect the endocrine system?

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Mosquitoes are well known as vectors for many pathogens, such as malaria (*Plasmodium falciparum*). Global warming and an increasing formation of potential breading habitats favor the global distribution of mosquitoes and pose a high risk to human health. Therefore, potent agents for the proper control of mosquitoes are indispensable. However, use of synthetic insecticides - such as DDT - bears the risk of causing serious damage to wildlife. As a consequence, there is need for alternative insecticides that effectively control pests while not impacting the environment. Over the past three decades a protein from *Bacillus thuringiensis israelensis* (*Bti*) has been successfully used as a biological control agent against mosquitoes. *Bti* is supposed to be ecological friendly, and thus, is used in ecological sensitive habitats. A recent study, however, has detected estrogenic activity in the *in vitro* Lyticase-supported Yeast Estrogenic Screen (LYES assay), after exposure to four different *Bti* formulations. Three formulations have shown significant estradiol equivalent quotients (EEQs) up to 22.8 ng/L. Subsequent studies revealed that the estrogenic activity was caused by the active substance rather than the compounds of the formulation matrix. To fully understand the mechanism by which *Bti* interacts with the endocrine system, further investigations are necessary.
The aim of this study was to analyze two *Bti* fermentation products, one of which has been proven to be active in the LYES assay, for additional endocrine potentials including disruption of steroidogenesis. *Bti* products of concern were extracted at two different temperatures (30 °C / 60 °C) using liquid pressure extraction. Extracts were then analyzed in the H295R steroidogenesis assay, an *in vitro* screening assay using a human adrenocortical carcinoma cell line. We focused on mayor hormones of the adrenal gland - such as estradiol, testosterone, androstenedione, progesterone, 17-hydroxyprogesterone and 21-hydroxyprogesterone - using LC-MS/MS and commercial ELISA kits to quantify hormone concentrations. Preliminary results indicate that both products have no significant effects on hormone production. Furthermore, we are currently

verifying the results from the LYES assay using a breast cancer cell line (MVLN). Both products showed an increase of human estrogen receptor (hER) binding at the highest concentration during a pilot experiment.

MO 141

Intersex in Scrobicularia plana: transcriptomic analysis reveals novel genes involved in endocrine disruption

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Successful reproduction is a vital process for the survival of any species. Xenobiotics that interfere with normal male and female gonad development will alter the population structure. In contrast to the extensive studies performed on vertebrates, there has been little information available regarding the gonad transcriptomes of molluscs. Our previous analyses on mussels revealed that a large number of genes showed sexually dimorphic expression in the gonads of adult and juveniles.
UK populations of the common estuarine bivalve S. plana are considered to be inherently gonochoristic and their extensive distribution, sedentary lifestyle and deposit feeding habit make S. plana a potentially valuable monitoring species. In this context it is interesting, therefore, that this species has been observed to display intersexuality (feminisation of males), including following exposure to known endocrine disrupting chemicals (EDC).
In order to identify and characterize putative effects of endocrine disrupting chemicals (EDCs) on gonad development and function of S. plana, we isolated candidate sex-specific transcripts using a SSH (Suppression Subtractive Hybridization) technique. The current paper describes some important and unexpected observations on the expression of sex related mRNA in these clams.

MO 142

Multi generational and individual effects of endocrine disruptors on growth and reproductive endpoints using the copepod, eurytemora affinis

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The watershed area of the Seine estuary is under high anthropogenic pressure due to high urban density, to an intensive industrial activity (mainly chemical industries) and also agriculture. Consequently, the Seine estuary is one of the most polluted area in the north of Europe. In addition, most of chemical compounds present in the Seine estuary are persistent threatening the health of organisms living in this environment. Troughs the generation, organisms are perpetually exposed to chemical and biological molecules. The evaluation of the quality of the Seine estuary has become a major issue in the last years, in particular on endocrine disrupter. The present work is to develop ecotoxicological tools for identifying reproductive and growth disrupting at the sub-individual, individual and populational level of a calanoïde copepod species, Eurytemora affinis.
To meet our objectives, we applied parallel handling multi-generational protocol and a bioassay based on embryo-larval growth and reproductive endpoints. At first after one generation of acclimatation, ovigerous females of copepods were exposed to a various chemical compounds (PCB126, 4-NP, methylfarnesoate) at a sub-lethal concentration then two generations were followed. For each generation, clutch size, individual number and stages were estimated. In parallel, new hatched of nauplii were exposed for 6 days to the same chemical molecules. Every 2 days mortality, growth and chitobiase activity were followed.
The results obtained from the experiments showed that the first generation is very sensitive to effects of contaminants. However, subsequent generations as well as lower juvenile stages seem to be much less sensitive. Following the results, it appears that copepod Eurytemora affinis is capable to adapt to its environment.

MO 143

Photosynthetic and proteomic responses of the marine diatom Thalassiosira pseudonana to triphenyltin exposure

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Triphenyltin compounds (TPTs) have been widely detected in the marine environment because of their widespread applications as antifoulants (e.g., on ship hulls and submerged mariculture facilities) and biocides against fungal diseases. However, little is known about its toxicity towards marine autotrophic species. Marine diatoms, as globally important primary producers, are responsible for 20% of global carbon fixation. It is, therefore, important to investigate if TPTs can pose hazard to marine diatoms. The marine diatom *Thalassiosira pseudonana* was the first chosen eukaryotic marine phytoplankton as model species for whole genome sequencing, and its available genomic information enables toxicologists to investigate the algal response to environmental contaminants at molecular levels. This study was designed to elucidate molecular toxic mechanisms of TPTCl on *T. pseudonana* by using an integrative approach of measuring physiological end-points (i.e., growth inhibition and photosynthetic response) and molecular responses (i.e., proteome expression). Through the standard growth inhibition test, we found that the 96-h EC50 value was 1.90 µg/L (95% CI: 0.96 - 3.78 µg/L). Using the pulse amplitude modulated (PAM) fluorometry, the 96-h EC50 values for photosynthetic parameters were founded to be 2.67 µg/L (95% CI: 2.50 - 2.84 µg/L) and 2.62 µg/L (95% CI: 2.44 - 2.82 µg/L) for Φ*P0* and Φ*P*, respectively. The results also showed that increasing exposure concentrations of TPTCl led to reduction in photochemical quenching (i.e., decreased Φ*P0* and Φ*P* values). This dwindling trend of both Φ*P0* and Φ*P* indicated that electron transport from photosystem II (PSII) to photosystem I (PSI) was hindered. Proteomic response of *T. pseudonana* is currently being investigated using two-dimensional electrophoresis and advanced mass spectrometry. As anticipated, the results of the proteomic analysis will be essential for revealing the toxic mechanisms of TPT on the diatom and identifying a suite of protein biomarkers as exposure and/or effect indicators.

MO 144

Mechanisms of action of the neural disruptor group 'selective serotonin reuptake inhibitors' in Daphnia magna

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Selective serotonin reuptake inhibitors (SSRIs) are known to increase offspring production in Daphnia magna. This study tested the hypothesis that the increase of serotonin post-synaptic activity by SSRIs changes the perception of the food environment and switches life-history responses towards higher food level: females reproduced earlier, producing more but smaller offspring. D. magna reproduction tests, respiration, feeding and survival-starvation assays and studies of lipids, proteins and carbohydrate levels of unexposed and exposed females to the SSRIs fluoxetine and fluvoxamine and the 5-HT serotonin receptor antagonist cyproheptadine. Factorial life-history experiments and reproductive assays showed that exposure to SSRIs increased juvenile development rate, clutch size and decrease offspring size at low and moderate levels of food rations. These effects were reverted by the presence of cyproheptadine, indicating that 5-HT function was essential to the SSRIs effects on Daphnia and linking them to the pharmacological effects of SSRIs in humans. Respirometry and survival assays and biochemical analyses on lipids, proteins and carbohydrate levels showed that SSRIs increased oxygen consumption rates and decreased carbohydrate levels in adult females. These changes did not effect survival under starving conditions, but they significantly affected the capacity of the exposed animals to survive under anoxic conditions. These results suggest that SSRIs increased aerobic catabolism in D. magna making exposed individuals apparently more fitted exploiting food resources under normoxic conditions, but at the cost of being more sensitive to low oxygen levels, a common situation in natural environments.

MO 145

Effects of chronic exposure to gemfibrozil on aquatic organisms Pseudokirchneriella subcapitata, Daphnia magna, Moina macrocopa, and Oryzias latipes

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Gemfibrozil is a commonly used lipid regulator in humans. Gemfibrozil has been frequently detected in the aquatic environment, and suspected for adverse ecological consequences not only because of frequency of detection but also its high log K_{ow} value (4.76). In this study, we conducted the chronic toxicity tests using freshwater algae *Pseudokirchneriella subcapitata* (72 hr), cladocerans, *Daphnia magna* (21 d), *Moina macrocopa* (7 d) and, 132 d long fish toxicity test using *Oryzias latipes*, and report the toxicity information that could be used for risk assessment of gemfibrozil in freshwater. In *P. subcapitata* test, the 72 hr EC_{50} was 5.27 mg/L (95% confidence interval of 4.77-5.62). In *D. magna* test, survival was reduced significantly at 5mg/L. In fish test, the body length of 30-day post hatch (dph) juvenile fish was significantly decreased at the gemfibrozil concentration of 3mg/L. When the mRNA expressions of several mRNAs related to endocrine disruption were measured at 30 dph juvenile fish, significant up-regulations of vitellogenin1 (vtg1) and vtg2, and cyp19β mRNA levels were observed in the juvenile fish at 3mg/L, suggesting effects on steroidogenesis and estrogenicity of gemfibrozil in fish. Histological observation at 50 dph revealed the presence of tubular basopilia and tubular vacuolization in kidney of the exposed fish . Our results demonstrate that long-term exposure to gemfibrozil resulted in adverse effects of survival and reproduction in cladocerans and fish. Mechanisms of endocrine disruption in fish warrant further investigation.

MO 146

Endocrine disruption effect of chronic exposure to mefenamic acid on aquatic organisms Daphnia magna, Moina macrocopa and Danio rerio

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Pharmaceuticals are trace contaminants of growing importance in aquatic ecosystem due to their physiologically active nature and their potential for impacts on non-target species. Mefenamic acid (MFA, CAS No. 50-78-2) is a non-steroidal anti-inflammatory drug (NSAIDs), which has been widely used for analgesic, antipyretic and anti-inflammatory purposes.We evaluated the acute and chronic toxicity of mefenamic acid employing several aquatic organisms, including two cladocerans, Daphnia magna and Moina macrocopa, and a teleost, Danio rerio.. The 48 h acute median effective concentration (EC_{50}) of D. magna was determined at 17.16 mg/L. In 21 d chronic toxicity test, D. magna showed significant changes in reproduction related characteristics after the exposure. In the early life stage test using D. rerio, there was a significant decrease of larval survival at as low as 1 mg/L of mefenamic acid. In addition, vitellogenin gene expression and VTG protein level were reduced at the highest experimental concentration of mefenamic acid, 1 mg/L. The result of this study indicates that this pharmaceutical may have a potential effect on survival, reproduction and growth of the aquatic

organisms, but the effect concentrations are a few orders of magnitude greater than those occurring in the ambient water environment.

MO 147

The effects of nonylphenol ethoxylates having different ethylene oxide (EO) chain on fish, daphnia, and alga

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Nonylphenol ethoxylates (NPEs) have been used as surfactants in detergent formulations in both of industrial and domestic. NPEs are biodegraded to shorter ethylene oxide (EO) or nonylphenol (NP). NP shows high toxicity to aquatic organisms, and also, NPEs having shorter ethylene oxide (EO) chain have been known to show greater toxicity than longer EO chain. Therefore, it is important to examine the effects of not only NP but NPEs on aquatic organisms. However, there were little toxicity data on aquatic organisms of different EO chains. To examine the different effects of NPEs having various EO chains (NP1EO, NP2EO, NP3EO, NP4EO, NP5EO, and NP6EO) on aquatic organisms, we performed the acute toxicity tests using alga (P. subcapitata), daphnia (D. magna), and fish (O. latipes). Each acute toxicity test was carried out according to OECD test guidelines No. 201, 202, and 203. Chemical analysis of NPEs concentrations in test water were carried out using LC-MS-MS.
In fish acute toxicity test, our results showed that NPEs having shorter EO chain had greater toxicity than that having longer EO chain. The toxicities were observed in range from 1 ppm to 5 ppm in LC50 (96 h). The similar results were shown in alga and daphnia. In the present study, the toxicity of NPEs was shown in all species examined. In further study, we need to compare toxicity among alga, daphnia, and fish for each NPE.

MO 148

Can fish embryos help predict endocrine disruption? An example with genistein

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The plant-derived isoflavone genistein is categorised as a weak oestrogen and the effects of genistein are well documented by many, particularly fish studies. However, these studies required the use of numerous animals, as do all current regulatory accepted tests for endocrine disruption. Hence, alternative methods need to be considered to comply with ongoing changes in regulation to fulfil the 3R's principle and reduce animal testing.
In this context, we studied the suitability of fish embryos for testing and analyzing endocrine disruption, using genistein as a model substance. Fish embryos are not regarded as protected animals even though their use allows effects to be assessed in a whole living organism. The drawback of fish embryos is that they are sexually undifferentiated and conventional endocrine disrupting adverse effects, like gonadal malformations or sex ratio alterations, cannot be assessed. To overcome this obstacle, we used transcriptomics to address suborganismic test endpoints.
We chose two complementing fish species in terms of embryogenesis time and sexual differentiation, zebrafish and medaka. For zebrafish, microarray experiments were conducted, whereas for medaka, gene expression of selected endocrine genes was analyzed by quantitative PCR. Functional gene enrichment analysis of the zebrafish microarrray data identified several affected pathways, including pro-apoptotic signaling and the disruption of brain and nervous system development. Hox genes were downregulated. Further, the estrogenic biomarkers *aromatase b (cyp19a1b)* and *vitellogenin (vtg1)* were already upregulated at low genistein concentrations (EC10), emphasising the high oestrogenic potential of genistein. These biomarkers had also been induced in medaka, additionally to species-specic responses, including *estrogen receptor 2a* gene induction.
In conclusion, the transcriptome response of zebrafish revealed key mechanism of genistein's molecular action, whereas with the medaka data, a more in-depth insight in the estrogenic mechanisms was achieved, making both fish species complemental. Overall, we demonstrated that combining fish embryo testing with transcriptomics emerges as a beneficial and animal free approach for testing endocrine disruption.

MO 149

Effects of the UV filter benzophenone-3 in adult zebrafish (Danio rerio) and eleuthero-embryos at environmental relevant concentrations

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Organic UV filters including benzophenone-3 (BP-3) are widely used to protect humans and materials from damage by harmful UV irradiation. These compounds enter the aquatic environment directly from sunscreen application, or indirectly via wastewater. BP-3 has been detected in surface water, wastewater and in biota. To date, still little is known about the fate and effects of this compound. BP-3 and some of its metabolites, which comprise of benzophenone-type moieties, were previously shown to have estrogenic effects in fish *in vitro* and *in vivo*. In our study, effects of BP-3 are evaluated after an exposure of adult male zebrafish (*Danio rerio*) and zebrafish embryos for 14 days and 120 hours post fertilization, respectively. Exposure concentrations of BP-3 are 10, 200 and 600 µg/L, as confirmed by LC-UV. The water analysis indicates that within 48 hours adult zebrafish, but not embryos, transform BP-3 in part to benzophenone-1 (BP-1), an estrogenic compound also used as UV filter. BP-3 and BP-1 are accumulated in fish up to 21 µg/g and 266 ng/g b.w., respectively. We analyse molecular effects by whole-genome transcriptomics (microarrays) and find no significant transcriptional alteration at 2.4 µg/L. At 312 µg/L BP-3, 123 transcripts are altered belonging to different pathways. By applying a target gene expression approach focusing on the endocrine system in the brain, liver and testis of adult zebrafish and in embryos, expression of estrogen receptor, androgen receptor, and vitellogenin are determined by qRT-PCR, as well as key enzymes involved in steroid hormone synthesis, such as the hydroxysteroid dehydrogenases, hydroxylases, aromatases. Transcript and protein level of vitellogenin is not induced up to 312 µg/L BP-3 in adult zebrafish (441 µg/L BP-3 in embryo). Our gene expression analysis data indicate that BP-3 has a low anti-estrogenic and anti-androgenic activity in adult zebrafish and embryos at environmentally relevant concentrations. The analytical chemical analysis emphasizes that effects may be related to a combination of the parent compound (BP-3) and its transformation products including BP-1.
The study was funded by the Swiss National Science Foundation (project No. 31003A-121829 to K.F.)

MO 150

Reversibility of endocrine disruption in zebrafish (Danio rerio) - comparison of different effect levels

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Endocrine disrupting chemicals (EDCs) exert effects at very low concentrations and can cause serious problems for the hormonal balance of various organisms. Exposure of wildlife to EDCs is not necessarily continuous, but may often occur in pulses. Consequently for the evaluation of the long-term effects on populations, it is essential to know whether such EDC-related effects are reversible. Three different substances selected for different modes of action were tested for their long-term impact on sex ratio, gonadal development, vitellogenin (VTG) induction and aromatase activity in zebrafish: the androgen trenbolone binds directly and very effectively to the androgen receptor. Ethinylestradiol, a synthetic derivative of estradiol, causes feminization in wildlife and humans. The fungicide prochloraz acts as an aromatase inhibitor by direct interference with the aromatization of androgens to estrogens. All compounds have previously been shown to cause striking effects in zebrafish, but recovery has never been studied in detail. In order to test whether EDC-related effects are reversible, an exposure scenario limited to 60 d was followed by (a) a recovery period of 40 d or (b) continued exposure for another 40 d. Four effects levels were examined: (1) population level: sex ratio; (2) organism level: growth; (3) organ/tissue level: histology of gonads (light microscopy); and (4) molecular level: vitellogenin induction (ELISA) and aromatase expression (RTq-PCR).
Results show clear correlation of effects at all levels, but clear-cut differences between the two different exposure groups. We conclude that endocrine disruption in zebrafish following discontinuous exposure is only partially reversible and may thus have serious implications for fish.

MO 151

Testing chemicals for endocrine activity by 21-day fish screening assay

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Beyond designed properties, plant protection products, biocides, pharmaceuticals and other chemicals may pose undesired impacts on aquatic environment via sewage. Endocrine Disrupting Chemicals (hormone-like) are toxicants that cause various effects in regulatory functions depending on length of exposure period, age, sex and stage of organism exposed. Testing chemicals for endocrine activity is required by law. For this reason, OECD Guideline for Testing of Chemicals No 230 (Sept 2009) introduced bioassay using endpoint biomarker - vitellogenin (VTG) in fish.
Zebrafish WT AB adults of both sexes were exposed for 21 days to four chemicals: E2, prochloraz, flutamide and propiconazole. VTG biomarker of endocrine activity was determined in whole body homogenates by ELISA and additionally gonadosomatic index (GSI) was reported. Results were analysed by ANOVA statistics. Natural estrogen E2 caused increase of VTG in males and prochloraz (fungicide, aromatase inhibitor) caused decrease of VTG in females. Therefore, positive controls confirmed correct test design. Changes of VTG level detected in female fish exposed to flutamide (nonsteroid anticancer drug) suggest U shaped concentration-effect curve. Decrease of GSI in male fish was also observed. VTG levels were increased in female and decreased in male fish corresponding with concentration of propiconazole (biocide, fungicide) whereas GSI in male fish was increased.
Evaluation of endocrine activity in in vivo models requires integration of processes in complex organism. Therefore, implementation of standard screening methods is expected by regulatory institutions and producers of chemicals.

MO 152

A comprehensive study on the toxicity of triphenyltin chloride to the rotifer Brachionus sp. at different biological organisation levels

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Phenyltin compounds in particular triphenyltin (TPT) are widely applied as effective biocides for different industrial and agricultural purposes. These compounds have been detected in the marine environment but little is known regarding their toxicity to the marine organisms. This study was designed to comprehensively investigate the molecular, individual and population responses of the rotifer, *Brachionus* sp. upon waterborne exposure to TPT chloride (TPTCl). Our results indicated that the population growth rate of the rotifers was decreased as TPTCl concentrations increased. A 96-h EC50 value for population growth inhibition was found to be 1.96 µg/L, which was ten times lower than the 96-h LC50 value derived from a standard acute toxicity test (i.e., 29.6 µg/L; 95% CI: 27.2 - 32.1 µg/L). At molecular level, gene expressions of twelve heat shock proteins (*hsp*), four glutathione S-transferases (*GST*), one retinoid X receptor (*RXR*) and thirteen cytochrome P450 monooxygenases (*CYP*) were studied for their responses to TPTCl exposure. At 20 µg/L TPTCl, hsp 90α2, *GST-O* and *CYP 29* were significantly up-regulated with the relative expression levels to the control up to 32.9, 4.4 and 62.6 folds, respectively. Temporal trends of these three genes were further studied in rotifers exposed to TPTCl over a period of 24-h. The expressions of these genes showed an increasing trend in the first few hours after TPTCl exposure, peaking at 3 h (for *hsp 90α2* and *GST-O*) and 12 h (for *CYP 29*) and then followed by a gradual decline. The overall findings of this study provide a better understanding on toxic mechanisms of TPT-mediated effects in the rotifer.

MO 153

Expression of all-trans and 9-cis retinoic acid receptor (RAR/RXR) genes during the zebrafish early development

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The zebrafish genome encompasses no less than 10 different genes codifying either for retinoic acid (RAR) or 9-cis retinoic acid (RXR) receptors, which participate in the retinoic acid response as well as in many other hormone-dependent regulatory pathways. In this work we analyzed the changes on mRNA abundance of each of these ten genes (RARaa, RARab, RARga, RARgb, RXRaa, RXRab, RXRba, RXRbb, RXRga, RXRgb) during the first 5 days of zebrafish development. The data shows a transition from maternal to embryonic transcripts during the first 24-48 hpf (hours post fertilization), as well as a differential response of the receptor genes to the exogenous addition of their cognate ligands, particularly during the first 24 h after fertilization. These results suggest that this transitional period between maternal to embryonic mRNA is particularly sensitive to the presence of putative disrupters (retinoids or rexoids), and that the RAR/RXR system is functional throughout the zebrafish eleutheroembryonic period. As several emerging contaminants are suspicious of disrupt either the RAR/RXR or other mechanistically related hormone regulatory systems (TR, CAR, PXR, PPAR, and others), the analysis of the retinoid/rexoid response in zebrafish embryos facilitates its implementation as convenient, non-animal model to assess these potentials risks.

MO 154

Sexual endocrine disruption in fish with focus on estrogen receptor antagonists- a fish life cycle test with fulvestrant

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Estrogen receptors represent important interfaces for mechanisms concerning gonadal development and reproduction of fish and therefore target sites for endocrine disruption.
Within the scope of establishing a tiered testing strategy to detect and assess a potential for sexual endocrine disruption in fish, data is needed to detect sensitive windows of exposure. Furthermore, the respective windows of effect manifestation should be identified. Especially for the estrogen receptor antagonists, a data gap is evident.
A full life cycle test was performed at the Fraunhofer IME to detect the population relevant effects of the selective estrogen receptor down regulator (SERD) fulvestrant on zebrafish. The nominal test concentrations were 1.3, 4.0, 13 and 40 µg /L. The test was performed under flow through conditions.
The test was initiated by introduction of fertilised eggs in the test vessels. The fish were kept until they have reached the adult stage. Survival, Growth and reproductive parameters were recorded. Secondly, a filial generation was prepared and effects on the early life stage phase (survival and growth) will be recorded.
A significant effect on reproduction could be observed at 13 and 40 µg fulvestrant/L. The cumulative number of fertilised eggs was found to be reduced.
The results confirm findings from a former study with the anti-estrogen tamoxifen-citrate, suggesting the sexual development as sensitive window of exposure and reproduction as sensitive window of manifestation for the estrogen modulated mode of actions.

A shift towards an increased number of males could be observed for tamoxifen-citrate. This has to be confirmed by dissection and sexing of the fish at end of the FLCT with fulvestrant.

MO 155

Peak exposure versus intrinsic toxicity in fish full life cycle tests with an anti-estrogen

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Environmental exposure is characterised by seasonally and locally fluctuating concentrations due to imission patterns, hydromorphology and dilution by rainfall events. Thus, the duration of concentration peaks surpassing effect threshold levels has to be compared with intrinsic chronic toxicity data, e.g. by calculating time weighted average concentrations. This is especially problematic when focussing on endocrine effects, as the most sensitive life stages or performances regarding effect setting and effect manifestation may be different. Both have to be covered by exposure and appropriate endpoints. For this reason, fish full life cycle (FFLC) or multi-generation tests are performed in flow-through systems with permanent exposure. These tests are not able to differentiate endpoints according to their susceptibility to short-term exposure and reversibility of effects. We perform FFLCs simulating worst case peak exposure by using static artificial sediment/water systems (270 L) with three life stages of zebrafish (fertilised eggs, juveniles, spawning adults) separated by stainless steel nets. The fish groups including their filial generation are investigated during declining exposure. Measured effects can be related to initial concentrations and to time weighted average concentrations during defined life stages.
There is still a data-poor situation for anti-estrogenic effects. In zebrafish, these are represented by a reduction of fertilisation rate and egg quality (exposed adults) and a sex ratio shifted towards males (fish exposed during sexual maturation). We used fulvestrant as potent anti-estrogen in a flow-through FFLC and a static peak exposure test with artificial sediment to
- confirm or add knowledge to population-relevant effects caused by anti-estrogens,
- compare effect threshold concentrations of peak versus permanent exposure,
- find principles of linking endocrine exposure and effects via bioaccumulation and/or stage-specific time weighted average exposure concentrations,
- assess the relative sensitivity of endpoints depending on exposure duration,
- rank endpoints according to their relevance for population effects.

In the peak exposure test the DT50 in the water column was measured to be approximately 0.5 d. The only effect was a temporary one on fertilisation rate at 632 µg/L (initial concentration) on days 4 to 6. The flow-through test at concentrations of 40, 13, 4 and 1.3 µg/L will be ended by the end of 2011.

MO 156

Characterization of the mode of action of the pharmaceutical clotrimazole on testicular steroidogenesis in zebrafish

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Clotrimazole is a pharmaceutical fungicide that has been recently detected in aquatic environment. This substance is known to inhibit CYP enzymatic activities, including several steroidogenic CYP but little is known about its in vivo endocrine disrupting potency in fish. In vertebrates gonadal steroidogenesis is under the control of the hypothalamus-pituitary-gonad (HPG) axis. The aim of the present study was (i) to assess the effect of clotrimazole on zebrafish testicular steroidogenesis by conducting in vivo and in vitro experiments and (ii) to characterize its mode of action by studying a network of functional target genes of the pituitary-gonad axis by means of Q-PCR.
In vivo exposures of male zebrafish to clotrimazole were conducted for 7 (70- 150 µg/L) or 21 days (20-200 µg/L) and led to concentration-dependent inductions of steroidogenic gene and protein expressions. In vitro testicular explants were exposed to similar concentrations of clotrimazole, and no effect was observed on transcript levels of steroidogenic enzymes. However, clotrimazole inhibited 11-KT release in the culture medium. This result suggests that clotrimazole does not act directly on testis to regulate the transcriptional activity of these genes. Induction of steroidogenic genes could be interpreted as a compensatory biological response to inhibition of cytochrome P-450 dependent steroidogenic enzymes.
To support this hypothesis, a network of functional genes of the pituitary-gonad axis was used. We showed that clotrimazole induce a cascade of molecular events in pituitary and testes. Transcript levels of genes encoding for pituitary Gonadotropin releasing hormone receptors (GnRH-R) and folliculo- stimulating hormone (FSH) -subunit, as well as testicular FSH receptor and steroidogenic enzymes were induced. All together, these molecular events are consistent with the involvement of FSH in inducing steroidogenic gene expressions to compensate the inhibitory action of clotrimazole on 11-KT synthesis.

Our study highlights the relevance of studying a network of relevant genes of the pituitary-gonad axis to investigate the mode of action of clotrimazole on the endocrine system of fish. Such approach could be extended to other compounds acting as inhibitor of P450-steroidogenic enzymes. The disruption of testicular steroidogenesis raises further concerns about the impact of clotrimazole on reproduction.

MO 157

Reproductive toxicity of methyltestosterone in embryo and adult zebrafish

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In Brazil, the hormone 17 α-methyltestosterone (MT), besides not being regulated is widely used in fish farming to reverse sexual juvenile females into male of tilapia. However, the effects of MT to non-target aquatic species and the environment are largely unknown. Field studies have documented physiologic and developmental abnormalities in feral fish, such as increased vitellogenin (Vtg) concentrations and gonadal intersexuality in male fish. Altered levels of Vtg have been widely used as an effective and sensitive biomarker for the detection of endocrine disrupting chemicals in the aquatic environment. The present work aims to assess the effects of commercial MT (cMT) (90% purity, Toledo, Paraná), as well as it's active ingredient 17α-methyltestosterone (aMT) (99.9% purity, Sigma) in adult and embryos of zebrafish (Danio rerio). Adults and embryos of zebrafish were exposed during 4 days to the nominal concentrations of 4, 23, 139, 833 and 5000 ug/L of both MT products. At the end of exposure adult fish were weighted and dissected to remove gonads and liver for further Vtg. Gonadossomatic (GSI) and hepatossomatic (HSI) indexes were determined in adult fishes. Results showed no significant differences in GSI neither in males or females exposed to cMT or aMT. The HSI was significantly higher in females exposed to the highest concentration tested of aMT and also in males exposed to the lowest concentration of cMT, suggesting that MT might induce hepatic toxicity, as expected since liver is the main organ for androgenic steroids metabolization. Hepatic and gonadal vitellogenin concentrations in adults did not show significant differences with cMT or aMT exposure. However, the Vtg levels in embryos were significantly lower in all concentrations tested of aMT and in two highest concentrations of cMT. These results suggest that MT might induce endocrine disruption in exposed early-life stages of zebrafish. In the other hand, the adult males and females that already have the endocrine system completely developed might be able to cope with MT stress as evidenced by the higher HSI registered. The lower levels of Vtg registered in MT-exposed larvae are in accordance with the reproductive changes caused by application of the hormone in fish farms to reverse sex in larvae tilapia. These results raise great concern about the risk of endocrine disruption caused by exposure to MT products of early life stages of aquatic non-target species.

MO 158
Sub-lethal effects of mixture of compounds in Zebrafish (Danio rerio)
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The prevalent use of different compounds in industry, agriculture, health care and other activities lead to an increased release of these compounds to the aquatic environments. Concerning the risk of mixture of these compounds in the environment, it is unlikely that fish are exposed to one single substance each time. There are few studies to evaluate the sub-lethal effects of mixture of different compounds on development stages, molecular physiology, and behavior of fish. Zebrafish, Danio rerio, is a suitable model in fish embryo toxicity test (FET) and behavioral studies. To evaluate the toxicity of mixture of compounds, the zebrafish embryos were exposed to single substances, including ethinylestradiol, nonylphenol, benzo-a-Pyrene, beta-nephtoflavone, and silver. The embryonic sub-lethal endpoints were heart rate, pigmentation, and eye development and the aim was to identify the most sensitive parameter. The lowest concentration of each single substance that might cause an effect (ECx) has been considered in joint mixture exposure. Since even the concentration below the threshold, which can cause no effect, might impair fish behavior, the movement of zebrafish larvae after 6 dpf (days post fertilization) has been studied. In molecular physiological level the induction of vitellogenin and CYP1A, in protein and gene expression levels, were measured in adult fish exposed to single compound and joint mixture to demonstrate the endocrine disrupting effects. Due to the interaction between the compounds in the mixture, there might be a cross-talk between estrogen receptor (ER) and Ah receptor (AhR) agonists available in the mixture of compounds that can inhibit or modulate the AhR- or ER- signaling pathways. Further, another sub-lethal effect, the multixenobiotic resistance, can be observed in fish exposed to the effluent of the sewage treatment plants for a long time. The present study has been undertaken to evaluate the sub-lethal effects of mixture of compounds on development, molecular physiology, and behavior of zebrafish.

MO 159
Zebrafish embryos as bioanalytical tools for detection of estrogenic and dioxin-like chemicals in environmental matrices
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Recent studies have reported the use of fish embryos as in vivo mechanism-based screening bioassays for the specific detection of biologically active compounds. In this study, we aimed at evaluating the use of zebrafish embryos for the detection of estrogenic and dioxin-like compounds in environmental matrices. Effect on phase I xenobiotic metabolism was assessed using EROD (Cyp1A-like) and BFCOD (Cyp3-like) assays in living embryos; estrogenic activity was measured using a transgenic zebrafish line expressing green fluorescence protein reporter gene under the control of the aromatase-B promoter (AroB-GFP). A panel of standards chemicals was first tested in order to calibrate the bioassays. One significant result was the finding that dioxin-like compounds were strongly active on the BFCOD assay. Then, these bioassays were applied to a multi-contaminated sediment extract, which has been shown to exert multiple toxicological activities as determined by a panel of in vitro bioassays. Both the crude extract and 4 fractions of increasing polarity (F1 to F4) and obtained from normal phase solid phase extraction were tested on the bioassays. Overall, crude and/or fractions were active on all endpoints, demonstrating the suitability of the bioassay to detect biologically active compounds. While no estrogenic activity could be detected in crude extract, weak activities were detected in F1, F2 and F3 fractions whereas in vitro estrogenic activity was only detected in F2 and F3. F2 and F3 are known to contain estrogenic compounds such as alkylphenols, parabens and steroids (data not shown). EROD and BFCOD gave parallel results, with significant activities in crude, and F1=F2>F3 fractions. Altogether these preliminary data show the suitability of zebrafish embryos-based assays to detect estrogenic and dioxin-like chemicals in environmental matrices and could serve as useful tools for effect-directed analysis approaches. Fundings: P189-ECOPI and ITN EDA-EMERGE.

MO 160
Evaluation of estrogenic activities of benzophenone derivatives using innovative in vitro and in vivo zebrafish models
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Benzophenone derivatives (BPs) are used as UV filters in many different products. These lipophilic compounds were recently described as ubiquitous contaminant of different compartiments of aquatic systems, including fish. In this study, we evaluated estrogenic activity of ten BPs in a model fish species, the zebrafish (Danio rerio), by combining newly developed in vitro and in vivo models. In vitro, three specific zebrafish reporter gene models expressing zebrafish estrogen receptors (ZfERs) in zebrafish hepatic cell line (ZFL) were used.Estrogenic activity of BPs was quantify in vivo by using a newly developed transgenic zebrafish line that expresses green fluorescent protein (GFP) under the control of the cyp19a1b promoter. The cyp19a1b gene codes for the brain aromatase B that is under the control of estrogens. Vitellogenin (Vtg), a marker of estrogenic compound, was used to assess the potential estrogenic effect of certain BPs in male fish.
Five of 10 BPs induced an estrogenic activity on the three models: BP2, THB, BP1, 4BP, while BP and 234 BP were non active. We noted diffrence in BPs ranking depending on the zfER subtypes suggesting receptor selectivity by certain BPs.
By quantifying GFP expression in live zebrafish, we confirm the estrogenic activity of some BP, i.e., BP1, THB, 4BP and 44'BP, as shown by their ability to induce GFP in a concentration-dependent manner. However, the ranking of BPs as a function of their estrogenic activity assay is different between models. For instance, 4BP was the most estrogenic compound in vivo but not in vitro. Differences were also noticed regarding the estrogenic activity of BP2. In vitro, BP2 has strong activity but had no effect on GFP in cyp19a1b-GFP embryo. However, BP2 induced strongly Vtg in male. The lack of estrogenic activity of BP2 in embryo may be related to difference of biodisponibility and/or metabolisation of this compound between embryo and adult fish. Our approach allows to characterize the estrogenic potency of emerging pollutants, using innovative in vitro and in vivo assays within a unique model fish species. The differences observed between assays deserve further studies to characterize the behavior of compounds in the different biological models in term of biodisponibility and metabolism.
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MO 161
Endocrine disrupting effects of OSPW and ozonated OSPW on sex steroid synthesis and signalling in fathead minnows
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There is concern about the large volume of oil sands process-affected water (OSPW) produced by surface mining of the oil sands deposits in Alberta, Canada. OSPW has endocrine disrupting effects on exposed fish and in vitro. Although ozonation attenuates some of the endocrine disrupting effects of OSPW the effects of ozone-treated OSPW on sex-steroid production and signaling in fish is unknown. In this study, sexually maturing male and female fathead minnows were exposed to either control freshwater, relatively fresh OSPW, or OSPW treated with 80 ml/L of ozone under conditions of static renewal for 7-days. At the end of the exposure period, brain, liver, and gonad samples were collected from each fish. Transcript abundances of 23 genes representing key signalling pathways and functional process of the HPGL axis were quantified by quantitative real-time PCR (qPCR). In male fathead minnow, abundances of transcripts of FSHb and LHb were greater in brains when exposed to OSPW compared to males exposed to freshwater. Ozonation attenuated the effects on abundances of transcripts of these genes. In testis isolated from males exposed to OSPW the abundances of transcripts of FSHR and LHR were greated compared to males exposed to the freshwater. Greater abundances of transcripts of ERa, VTG, CHGL and CHGH in livers from male fathead minnows exposed to OSPW suggested that some component of OSPW acted as an agonist of the ERa that stimulated signalling. In female fathead minnow, abundances of transcripts of of LHb but not FSHb were greater in brains when exposed to OSPW. Ozonation attenuated the effect on LHb but stimulated greater abundance of transcripts of FSHb. The abundances of transcripts of FSHR, LHR and CYP19a were significantly less in ovaries from females exposed to OSPW and ozonated OSPW compared the controls. The abundances of transcripts of AR, ERa, ERb, as well as the estrogen-responsive genes VTG, CHGL and CHGH were less in livers from females exposed to OSPW relative to abundances in livers form females exposed to freahwater. In sum, OSPW has endocrine disrupting effects all levels of HPGL axis in fathead minnows. OSPW has different effects in male and female fathead minnows. The results of varied effects may provide mechanistic basis for results from other studies. Ozonation attenuates affects of OSPW on some endocrine endpoints, and the effect is more prominent in males than in females.

MO 162
Differences in fathead minnow fecundity using tiles with and without trays for fish endocrine assays
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A trial to further evaluate the use of trays with tiles for the FISH SHORT-TERM REPRODUCTION ASSAY WITH THE FATHEAD MINNOW (Pimephales promelas) (FSTRA) test. The five-week trial simulated the experimental design of the FSTRA test that has a two-week pre-exposure period followed by a three-week exposure period. No test substance was used in the trials. Fish were divided into two test groups, one with tiles only and the other with tiles and trays. The test compartments followed the FSTRA guidelines and had three tiles per tank and reproductive groups that consisted of six fish (4 females and 2 males). Fecundity was measured daily throughout the five-week exposure. The methodologies used in the trials were those presented in OPPTS and OECD guidelines. The data for the first two weeks of the trial simulated the pre-exposure phase of the assay. The tile only group had a mean fecundity of 30.35 eggs per female per day and a CV of 35.6%, while the tile and tray group had a mean of 36.93 eggs per female per day and a CV of and 34.25%. This indicates that for the first two weeks, trays do slightly increase mean fecundity, but both groups clearly exceed the guideline requirement of 15 eggs per female per reproductive day and have similar CV's. The data for weeks 3 to 5 of the trial simulates the exposure phase of the test. The tile only group had a mean fecundity of 19.66 eggs per female per day and a CV of 26.7%, while the tile and tray group had a mean of 27.95 eggs per female per day and a CV of 42.8%. Fecundity in weeks 3 to 5 was greater for tanks having tiles with trays, however, the variability was much higher for trays and tiles which had a much larger CV. Of greater concern was that two of the tanks stopped spawning in the tile and tray group. One tank had 51.8 eggs per female per reproductive day during the first two weeks and zero for weeks 3 to 5, and the other decreased from 17.8 to zero eggs per female per reproductive day. Both of these tanks would likely qualify for inclusion in a test that would greatly confound the interpretation of the results. There also was a greater incidence of injuries with trays than without trays, which is supportive of our concern for injury from the trays and screens in tanks. The use of trays with tiles in fathead minnow reproduction tests does increase fecundity, but increased variability in the last three weeks of a five week trial.

MO 163

Reproduction and endocrine function in Fathead Minnows (Pimephales promelas) exposed to Polybrominated Diphenylether (DE-71)

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To determine if DE-71 altered reproduction and endocrine function in fish, the Tier 1 EDSP 21-day Fish Reproduction Screen with fathead minnow (Pimephales promelas) was used. Reproductively-active male and female fish were exposed to DE -71 (0 [control], 0.65, 1.3, 2.5, and 5.0 µg/L) via flow-through exposure for 21-d and evaluated for survival, reproductive behavior, and secondary sexual characteristics. Reproductive fecundity and fertilization success were monitored daily. At termination, the status of the reproductive endocrine system was assessed by the gonad-somatic index (GSI), gonadal histology, plasma steroids (estrogen [E2] and testosterone [T], and 11-ketotestosterone [11-KT]), hydroxysteroid dehydrogenase [HSD], and plasma vitellogenin (VTG). Results indicated that the DE-71 exposure did not affect survival or body weight, but reduced male GSI. Reproductive fecundity, gonad histology, and endocrinological measures of reproductive status were altered. Exposure to DE-71 did not alter plasma E2 and VTG levels in females, however; decreased plasma T levels were detected in both sexes. These results were generally similar to those found in S. tropicalis during gonad differentiation demonstrating similar effects of polybrominated diphenylethers on the reproductive system of male fish. Evaluation of HSD activity and the male-only androgen 11-KT will be presented to describe whether the effect may be related to general alteration of early steroidogenesis as measured by HSD, or if DE-71 is more specifically altering androgenesis in male fathead minnows as measured by 11-KT and thus, acting in an anti-androgenic manner.

MO 164

Endocrine disruptive effects of the common feedlot contaminant 17a trenbolone on the Australian Murray River rainbowfish (Melanotaenia fluviatilis)

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The effects of Endocrine Disrupting Chemicals (EDCs) are of global concern; however in Australia their potential effects are largely unknown particularly on native species. In Australia, the beef industry is largely dependent on Trenbolone acetate (TBA) implants, a synthetic steroid that is used as a growth promoter. Within the animal's body the administered acetate is hydrolysed to 17β trenbolone and part of this one epimerized to 17β trenbolone. In animal wastes the proportion of the isomeric form α is estimated to be 10 fold higher than β, where these metabolites are known to be very stable. The aquatic environment is potentially exposed via direct discharge, runoff, or both. This study evaluated the androgenicity of 17α trenbolone on the native Australian Murray River rainbowfish, Melanotaenia fluviatilis. Four adult female fish and two male fish per tank were exposed for 21 d to three different concentrations of 17 α trenbolone. Cumulative egg production, hatchability, larval fitness as well as adult VTG concentrations and histopathology of gonads were assessed. In vivo exposures at the tested concentrations lead to the masculinisation of the female fish at the highest concentration tested. Fecundity of the fish seems to be reduced as well as larval fitness, leading to deformities in new hatched larvae. Gonadal morphology of adult female fish also seems to be affected by the exposures.

MO 165

Effects of towel eluates on Vitellogenin levels and EROD activities in rainbow trout (Oncorhynchus mykiss)

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The consumption of textiles in the world is increasing every year. Several chemicals used in textile industry and fabrics may have adverse effects on aquatic organisms. Alkylphenols like Nonylphenol (NP) are one of the widely used chemicals acting as a dispersing agent of color pigments in the textiles with a high amount of outlet in the aquatic environment through industrial and household waste. NP is reported to have estrogenic activity in both in vitro and in vivo studies. Limited studies have focused on the estrogenic activity of chemicals present in towels. To evaluate the estrogenic activity of chemicals present in towel eluates juvenile rainbow trout were exposed to waters from heated towels and "filtered"towels for 6 days. Induction of vitellogenin (VTG) protein, a biomarker of exposure to xenoestrogen, was observed in the fishes exposed to water from heated towel but surprisingly in fishes exposed to "filtrated"towels the VTG levels were suppressed. The possible effects of these exposures on the CYP1A activity (EROD activity) showed a drastic increase of hepatic CYP1A activity in fish exposed to filtrated towels but lower CYP1A activity in fish exposed to heated towel water. It should be noted that textiles contain complex mixture of compounds, possibly containing both VTG and EROD inducing chemicals. There might be Ah receptors agonists in filtered towel water which can induce EROD activity, while they can suppress the induction of VTG. On the other hand, since there is a high EROD activity in this group, ER agonists could not inhibit the induction of CYP1A gene expression. This might be explained as a one-way inhibition AhR-ER cross-talk when the fish were co-exposed to AhR and ER agonists. The difference between the response in heated and filtered eluate exposure may be due to volatile Ah receptor agonist evaporated from the eluate. The present study was undertaken to evaluate the estrogenic activity of towel eluates in rainbow trout and also the effects on EROD activities. The study was conducted as a student project in the Master course Ecotoxicology with emphasis on physiology at the University of Gothenburg, Sweden.

MO 166

Effects of 17-β estradiol on thymus volume and regionalisation in juvenile sea bass (D. labrax L.)

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Providing the first lymphocytes during the maturation process of the fish immune system, the thymus is in addition to the head kidney considered to be a primary immune organ. It consists of two different compartments: the cortex and medulla. Immature T-lymphocytes migrate from the cortex into the medullary region during their maturation process. Only mature T-cells appear in the medulla. Contrary to mammals, there is no observable thymic atrophy in adult fish and the organ stays active during the whole lifetime. The critical period in thymic regionalisation lies between 51 and 92 dph in sea bass. The thymus gland is considered to reach adult volume 365 dph. The thymus is particularly susceptible to waterborne pollutants as only an epithelial layer separates it from the gill chamber. In mice it is evident that 17-β estradiol (E2) plays an important role in T-cell maturation, more precisely on the initiation of apoptosis in auto-reactive T-lymphocyte precursors, which occurs at the border between the two thymus regions. As a result of livestock breeding and anthropogenic wastewaters, higher concentrations of oestrogens are present in the aquatic environment, therefore the current study aimed to elucidate the possible impairments of E2, as a model oestrogen, on fish thymus.
Juvenile sea bass (D. labrax, 60 dph) were exposed to different environmentally relevant concentrations of E2 (0; 2; 20; 200 ng/L) for 56 days. The head sections, including the thymus, were prepared for histological observations in order to assess thymus volume, region volumes and the ratio between cortex and medulla. No differences in thymus volume or regionalisation between exposed (200 ng/L) and control fish could be observed. Nevertheless, E2 might affect the thymus at a sub-cellular level with consequences for whole organism immunity. For instance, we investigated the expression of different cluster of differentiation (CD) -receptors associated with T-cell maturation in a subsequent study. This research is funded by INTERREG IV A (DIESE, #4040) of the European Union.

MO 167

17-β estradiol impairs head kidney leucocyte phagocytosis in juvenile sea bass (D. labrax L.)

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With the detection of oestrogen receptors in immune relevant organs and cells, it seems likely that the functionality of the immune system is also dependent on the concentration of sex hormones in the organism. Knowing that the concentrations of steroid hormones are elevated in the aquatic environment, the question of effects on the immunity of aquatic animals arises. Exposure possibly leads to direct as well as indirect consequences on the mature immune system of adult fish. But more importantly, the development of the relevant immune organs may be impaired in larvae and juveniles.
Phagocytosis is one of the crucial functions of the innate immune system, and is one of the rare, established biomarkers for the immune system in ecotoxicology. Intracellular digestion of pathogens is followed by antigen processing and presentation, and the secretion of cytokines, which activates immune cells and the adaptive immune response. Here we investigate the impact of 17-β estradiol (E2), one of the most potent (xen)oestrogens, on the phagocytosis of head kidney leucocytes from juvenile Dicentrarchus labrax. Sea bass, at different developmental stages of the immune system (30 dph, 90 dph, 120 dph), were exposed to 20 ng/L E2 for 35 days. Phagocytosis of head kidney leucocytes was determined by incubating them with fluorescent latex beads and detecting cells with ingested beads via flow cytometry. Compostion of cell populations, mortality and phagocytosis were measured for the whole, lymphocyte and monocyte/macrophage populations. While no effect in phagocytotic performance was found in younger animals, we observed a significant difference for whole cell population and lymphocyte phagocytosis in the 120 dph group. Our results suggest that lymphocytes are more sensitive to E2 exposure than monocytes/granulocytes, where only a tendency towards a decreasing phagocytotic activity for exposed fish was found. As sea bass head kidney lymphocytes are mainly B-cells, the obtained results strengthen the observation of phagocyting B-lymphocytes in teleosts. The impairment of phagocytosis by an environmentally relevant concentration of E2 in nearly immune mature sea bass leads to the question of a potential impact on cytokine release and other B-lymphocyte

functions. Further these results indicate a possible impact on the recruitment of the European sea bass population, given the fact that European estuaries, serving as nursery areas, suffer from higher levels of oestrogen pollution.

MO 168
A non-invasive method based on head morphology to sex mature three-spined Stickleback (Gasterosteus aculeatus) in rearing conditions
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The threespine stickleback (Gasterosteus aculeatus) is a small-bodied teleost fish which is a major component of shallow water food webs in the northern hemisphere. G. aculeatus is a reference species for experimental studies, in particular for the assessment of endocrine disruptors. Sex ratio can bias the outcomes of an experimental study, especially if this study focuses on reproduction or behaviour. Moreover, sex-ratio, by itself, can be a very relevant endpoint in experimental tests. A mathematical model to distinguish mature female and male three-spined Sticklebacks G. aculeatus is proposed. This method is based on sexual dimorphism in the head morphology. The discrimination was established on five distances of interest on the head, divided by the standard length of fish. The parameters were estimated based on a training set composed of 102 fish and characterised by an equilibrate sex ratio and validated on a test set composed of 69 fish. Our model permits to balance between the percentage of fish that can be sexed and the percentage of fish correctly sexed. Compared to other available methods to sex G. aculeatus, our model is non invasive, not expensive, rapid, replicable, and can be calibrated out of the breeding period.

MO 169
Effects of produced water from an offshore oil-platform; an in vivo study using the three-spined stickleback (Gasterosteus aculeatus) as a model species
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There is growing concern over the high levels of anthropogenic contaminants entering the Arctic region. In light of the anticipated expansion of oil exploration and production in Arctic areas, of particular concern is the potential impact of hydrocarbon-related contaminants on the Arctic ecosystems. Several of these compounds are known to exhibit endocrine disrupting properties. The predicted expansion of oil production into Arctic areas would pose a considerable environmental risk, and highlights the need for the implementation of robust indicator species for future biomonitoring programmes.

The three-spined stickleback (*Gasterosteus aculeatus*) is a small teleost fish widely distributed throughout the Northern hemisphere, occurring as far north as Svalbard. This ubiquitous species is increasingly being recognized as an emerging model in ecotoxicology, notably as a sentinel for endocrine disruption. The stickleback can be used as a combined biomarker of both estrogenic and (anti-) androgenic compounds, and with the sequencing of its genome an increasing number of molecular tools are being developed for the assessment of contaminant exposure. The stickleback has the potential of becoming a valuable indicator species to identify and monitor the impact of anthropogenic pollutants in Arctic ecosystem, and be included in future biomonitoring programmes.
The objective of this study was to evaluate the effects on stress tolerance in fish after exposure to produced water, using the three-spined stickleback as a model organism. Effects were assessed by quantification of gene expressions (UDPG, CYP1A, VTG , PLA), in addition to measuring the levels of glucose and cortisol.

MO 170
ZnO nanoparticles exposure alters transcriptomic profile in Hydra
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The acute toxicity test for 20 nm ZnO and 100 nm ZnO and comparative transctriptomic profile analysis using hydra exposed to 20 nm ZnO and 100 nm ZnO were carried out. As a result, the LC50 for 72 hours was 8.7 mg/L in 20 nm ZnO exposure and 14.9 mg/L in 100 nm ZnO exposure group. For the microarray experiment we exposed hydra to 20 nm ZnO and 100 nm ZnO as the concentration of 1/50 of LC50 for 12 hours and hybridized those RNAs extracted from the exposed groups with that of control group on the hydra cDNA chips including 17,639 genes. As the results, 137 genes expressions were induced and 106 genes were reduced over 10 fold by 20 nm ZnO exposure. Among them the expression of multidrug-Resistance like Protein 1 CG6214-PM gene increased over 100-fold. In 100 nm ZnO exposure, the expressions of 137 genes were induced over 10 fold and 106 genes were reduced over 10 fold. The upregulated more than 2-fold in both 20 nm and 100 nm ZnO exposures were 886 genes and most of them belonged to cellular processes and signaling category and especially they were related to signal transduction mechanisms. The downregulated more than 2-fold in both 20 nm and 100 nm ZnO exposures were 1006 genes and most of them were related to signal transduction mechanisms. The functional clustering of differentially expressed genes by ZnO nanoparticle exposure showed that those nanoparticles tend to affect the transcription of genes in cellular processes and signaling group in most.

MO 171
Bioaccumulation and sublethal toxicity of 4-nonylphenol in chironomus riparius meigen 1804 (Diptera, chironomidae) larvae: assessment of mentum shape variations by means of morphometric analysis
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Nonylphenol ethoxylates are surfactants widely used to produce oil-soluble detergents and emulsifiers. In the environment these substances are transformed by microorganisms to form more toxic compounds, such as short-chain nonylphenol ethoxylates and 4-nonylphenol (4-NP), well known for their ability to mimic steroid hormones. In this work, we studied bioavailability, bioaccumulation and sublethal toxicity of 4-NP by exposing first to four instar chironomid larvae (*Chironomus riparius*) to a 4-NP-spiked sediment (0.5, 67.1 and 184.6 mg/kg d. weight). 4-NP in pore-water was monitored by Semi Permeable Membrane Device (SPMD). After 20 days exposure, larvae were removed and 4-NP concentrations in chironomid bodies were determined. On the head capsule, sublethal effects were assessed by observing and comparing four mentum shape responses: (1) rate of deformities; (2) the fluctuating asymmetry level via traditional morphometrics; (3) this same fluctuating asymmetry level via geometric morphometrics; and (4) subtle shape variations between the control group and stressed groups by means of geometric morphometrics. The bioaccumulation test revealed that the 4-NP uptake in organisms increased with increasing 4-NP concentration in pore water. Nevertheless no correlation could be drawn with either deformities or both FA indexes. Significant shape variation, corresponding to lateral tooth size increases, were detected at 184.6 mg/kg d. weight.

MO 172
Yolk proteins as biomarker for endocrine disrupters in bivalve molluscs
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Endocrine disrupting compounds (EDCs) are known to cause intersex and altered sex ratios in fish but effects of endocrine disrupters on bivalve molluscs have only been reported a few times. Vitellogenin, the precursor of yolk proteins, is a widely accepted biomarker for endocrine disrupters in fish as it is influenced by changes in circulating 17β-oestradiol (E2) levels. Yolk-like protein levels in bivalve molluscs have so far been determined by an alkali-labile phosphate (ALP) measurement assay, which is an indirect method for detection of yolk proteins and due to the unspecific character of the assay, it has been discussed whether yolk proteins are present in the hemolymph of bivalves and if production of yolk proteins in bivalves is induced by oestrogens and EDCs. A direct method for detection of yolk-like proteins in bivalves is therefore highly needed and we started development of an ELISA (Enzyme-linked Immunosorbent Assay) for yolk protein in bivalves as we have previously developed ELISAs for yolk protein in several fish species. Yolk protein levels in different bivalve tissues were determined both by ALP and the developed ELISA and a comparison of results obtained from both methods was made. In addition, swollen river mussels (Unio tumidus) were exposed to E2 (57, 164 and 512 ng/L) for seven weeks during the reproductive period to investigate if intersex could be induced. Histological examination of the gonads revealed that intersex could not be induced at these E2 concentrations and the presence and quantity of yolk protein in tissue and hemolymph was investigated.

MO 173
Comparison of vas deferens and penis development between the rock shell, Thais clavigera (Muricidae) and the ivory shell, Babylonia japonica (Buccinidae)
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The characteristics of the development of male genitalia (penis and vas deferens) in imposex-exhibiting female and male rock shells, *Thais clavigera* (Muricidae), were histologically examined using specimens from wild populations and tributyltin (TBT)-exposed females in the laboratory. Vas deferens and penis development was already observed in both imposex-exhibiting female and male rock shells even at approximately 6 months old. A variety of vas deferens morphogenesis patterns were observed in wild adult female *T. clavigera*, and the characteristics were summarised. The immature vas deferens at an initial stage, however, was only observed beneath or behind the penis, and no vas deferens was observed close to the vaginal opening (i.e., vulva) of the capsule gland in TBT-exposed females, which was different from the characteristics of vas deferens formation observed in wild females. Taking into consideration both the observed results from wild female specimens and from TBT-exposed females in the laboratory, the vas deferens sequence (VDS) index for *T. clavigera* was proposed as VDS 1-6. Meanwhile, we also histologically examined development of genitalia in the ivory shell, *Babylonia japonica* (Buccinidae), using 2-year-old shells from wild populations and laboratory-reared juveniles for 0-20 months of age. Differentiation of gonad (i.e., testis and/or ovary) was unclear before 14 months of age, and progressed after 16 months of age. Immatured vas deferens, however, was observed in males at 14 months of age, although no penis was observed in them. Formed penis was recognized in almost all males at 16 months of age, although vas deferens was not yet completed. Vagina, bursa copulatrix and capsule gland were developing in 14-month-old females. Albumen gland and receptaculum seminis were also developing in 16-month-old females. Differentiation and development of gonad did not precede the development of genitalia in the ivory shell, suggesting that regulatory mechanism of reproduction might be different between mollusks (prosobranch gastropods) and vertebrates. Moreover, there might be a considerable degree of difference on vas deferens and penis development

between the rock shell, *T. clavigera* (Muricidae) and the ivory shell, *B. japonica* (Buccinidae), namely, even among prosobranch gastropod species.

MO 174
Impact of Roundup® and 17a-Ethinilestradiol exposure on the liver morphology of bullfrog's tadpoles (Lithobates catesbeianus)
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Ectothermic vertebrates have melanocytes on several organs (lung, heart, thymus, and gonads) and tissues (meninges and connective tissues surrounding blood vessels), constituting an extracutaneous pigmentary system. Our results showed that both Roundup® and 17α-Ethinilestradiol provoked an increase in the liver pigmentation due to the patent increase of melomacrophages and MMG when compared to their respective controls. The melanomacrophages are pigmented cells with macrophagic activity. They are found in hematopoietic organs and even in the liver of amphibians and have different types of granules in the cytoplasm, besides melanin, that suggest the presence of chemically distinct substances. The functional role of these visceral melanocytes is unknown, but studies in low vertebrates like fishes and also in frogs showed that the melanomacrophages are evolved in inflammatory combat against bacterial and all kind of toxic substance. These cells are present in the liver of the adult amphibians under normal conditions, but present a considerable increase under toxic conditions. This process is so drastic that the change on liver pigmentation due these cells is the first step to analyze the liver response against inflammation. They do not only increase in number, but also form melonomacrophages aggregates (MMG). MMG are supposed to be a natural immunity and physiological response of low vertebrates against several toxic substances, bacterial infection and other antigens. Studies dealing with the effect of the cadmium in adults of Rana ridibunda showed the same results obtained here [3]. We also observed invasion of abundant immunity cells among the hepatocytes in exposed tadpoles. According to the authors, the melomacrophages may act as cell storage of toxic substances. The macrophages are able not only to accumulate metals and philological active molecules, but also are antigen-presenting cells that play a key-role in immunity system of vertebrates. As the mammalian macrophages, the frog melonomacrophages also accumulate hemosiderin by destruction of senescent erythrocytes. In this manner, the increase of the melanomacrophages and MMG in bullfrog tadpole exposed to Roundup® and 17α-Ethinilestradiol in the livers demonstrate a response to an inflammatory condition, which may jeopardize the development of the individual if in natural conditions the exposure to these xenobiotics are constant and maintained.

MO 175
Validation of the amphibian metamorphosis assay for potential endocrine disrupting chemicals with Xenopus laevis
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The new European Union Plant Protection Products Regulation (PPPR 1107/2009) identifies the need to consider whether a substance is a potential endocrine disrupter in aquatic non-target organisms and the current draft of the PPP data requirements refers to three screening assays for ecotoxicological endocrine-disrupting potential. Of these, we describe in detail our experience in the establishment and validation of the amphibian metamorphosis assay (OECD 231) with the African Clawed Frog.
In this method, in order to satisfy validity criteria in the rearing phase, conditions necessary to allow tadpoles to develop from fertilisation to development stage 51 as defined by Nieuwkoop and Faber (1994) were established, and individuals selected for the exposure phase and transferred to test vessels. To establish the assay, 400 tadpoles were exposed to a range of levels of the three reference substances, thyroxine (T4) which produces stimulatory effects on the normal function of the hypothalamic-pituitary-thyroid (HPT) axis, sodium perchlorate (which retards development) and iopanoic acid (which affects hind limb development) and levels of each were verified using an appropriate analytical method. At Day 7, 80 randomly selected individuals at each exposure level were removed and assessed (body weight, developmental stage, hind limb and snout to vent length). Exposure continued for a further two weeks and the study terminated on Day 21 when all the remaining individuals were assessed as on Day 7. Following developmental stage matching, 80 individuals were selected for thyroid removal and histopathological analysis.

We found that our results were similar to the ring test results published by the OECD (Series on Testing and Assessment Document Number 77) and make a number of observations on methodology that may improve the reproducibility of these assays.

MO 176
Progestins - potent endocrine disrupters of the female reproductive system
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Progesterone signalling has received very little attention as a potential target for disruption although it is a key regulatory pathway in the development and function of the female reproductive organs. Recent research has shown that progestins (synthetic progesterone) in the environment might pose a threat to egg laying in wild fish. Progestins are extensively used in contraceptives and in other hormonal therapies in human and veterinary medicine. More information on the targets and effects of progestins in adult and early life stages is needed to assess the environmental risks of this type of compounds. The main objective of this study was to determine developmental and reproductive toxicity of a common environmental progestin, levonorgestrel. Using the amphibian model Xenopus tropicalis (African clawed frog), effects of levonorgestrel on gonadal differentiation, reproductive organ development, oogenesis (egg development), spermatogenesis and fertility were characterized following developmental (larval) or adult exposure via the surrounding water. The test concentrations ranged from low environmentally relevant at 1 ng/L up to 1240 ng/L. Developmental levonorgestrel exposure inhibited oogenesis and caused a complete lack of developed oviducts which was visible in adult females. As a consequence, the females were sterile. No developmental effect was visible at metamorphosis, directly after the levonorgestrel exposure had been discontinued, implying that a full life-cycle study seems necessary to reveal the consequences of developmental exposure to this type of compounds. Also adult exposure to levonorgestrel inhibited oogenesis, implying impaired fertility. The lowest tested concentration,1.3 ng/L, increased the proportions of previtellogenic oocytes and reduced the proportions of vitellogenic oocytes in the ovary, indicating inhibited vitellogenesis. No developmental or reproductive effects of levonorgestrel were seen in the males. In conclusion, 1) the female reproductive system was more susceptible to progestin toxicity than the male system, 2) several stages of egg development (germ cell progression into meiosis and vitellogenesis) as well as the differentiation of the Müllerian ducts (precursors of oviducts) are sensitive targets for progestagenic endocrine disrupters.

MO 177
Biotransformation of PBDE-47 by human liver microsomes and Cytochrome P450s and formation of potentially toxic metabolites
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During the past decade both animal and human studies have supported an association between polybrominated diphenyl ether (PBDE) flame retardants and neurobehavioral / neurodevelopmental disorders, particularly following in utero and postnatal exposure. Evidence is also growing suggesting that bioactivation by oxidative metabolism adds considerably to the neurotoxic potential of PBDEs. Thus, there is a critical need to further our understanding of PBDE metabolism in humans. This study conducted a qualitative and quantitative characterization of the in vitro metabolism of 2,2',4,4'-tetrabromodiphenyl ether (BDE-47), the most abundant congener retained in humans, using recombinant human cytochrome P-450s (CYPs) (20 µM BDE-47) and pooled human liver microsomes (0.1 to 10 µM BDE-47). Of the 11 human CYPs that were screened, CYP2B6 was the predominant CYP capable of forming six different mono-hydroxylated-BDEs (OH-BDEs), s, including 3-OH-BDE-47, 5-OH-BDE-47, 6-OH-BDE-47, 2'-OH-BDE-66, 4-OH-BDE-42, and 4'-OH-BDE-49. With the exception of 2'-OH-BDE-66, all of these metabolites have also been detected in human blood samples, supporting the similar in vivo biotransformation of BDE-47. Moreover, the analysis by full scan GC/MS of the metabolites of BDE-47 formed by CYP2B6 showed the formation of di-OH-BDE-47 and di-OH-dioxin, a novel metabolite. Kinetic studies of BDE-47 metabolism by CYP2B6 and pooled human liver microsomes found Km values ranging from 1-2 µM, indicating the high affinity of CYP2B6 for the formation of hydroxylated metabolites. The prominent role of CYP2B6 in the metabolism of BDE-47 to potentially toxic metabolites will better inform future mechanistic and epidemiological studies investigating the potential of BDE-47 and its' metabolites to produce neurobehavioral / neurodevelopmental disorders.

MO 178
Affect of EDCs on fish communities in the Levuvhu River, Limpopo Province, South Africa
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Contaminants present within aquatic ecosystems worldwide are the result of agricultural applications, urban development and industrial effluents. Current contamination by DDT in the Luvuvhu River, Limpopo Province, South Africa is primarily due to IRS (indoor residual spraying) for mosquito vector control of the malarial epidemic. DDT and its resulting metabolites DDE and DDD may continue to persist in various environmental phases, long after spraying. The characteristically high lipophilicity, chemical stability and very slow biodegradation result in a high uptake or bioaccumulation. Despite DDT spraying for many years, limited data on these concentrations in aquatic ecosystems exists. Fish community structures are widely used to assess the effect of human impacts on aquatic ecosystems e.g. water quality, habitat deterioration and organism health. A study was therefore done to assess the effect of DDT, its metabolites and other pollutants in the water, sediment and biota in the aquatic ecosystem of the Luvuvhu River catchment.
Values for physico-chemical variables were measured to determine water and sediment quality. Available historical water quality data were obtained. Pesticides extracted from water, sediment, and fish tissue were quantified on a gas chromatography mass spectrophotometer (GC-MS). Electronarcosis and seine nets were used for fish sampling from different river habitats. Frequency of occurrence and relative abundance of fish, and non-parametric diversity indices were determined. Relative abundance for fish communities were described employing two statistical models. Selected biomarkers were used to determine sub-cellular effects of EDCs in field sampled fish.
Extensive abstraction of water occurs for irrigation, aforestation, community development and extensive rural activities in the in stream and riparian habitat. These activities yielded impacts such as bank erosion, flow modification, water quality changes, bed modification and some solid waste disposal. Pesticide levels were only above existing guidelines at specific sampling sites. Biomarkers showed effects of the contaminants on sub-cellular to organ levels with no effects on organism survival. No changes in fish community structures occurred while exposed to DDT and other contaminants measured in the study. The exposure duration and/or concentrations of pollutants were probably too low to induce any effects. Ecosystem services are therefore not negatively impacted.

MO 179

Distribution of endocrine disrupting pollutants in the Long Island Sound

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Waste water treatment facilities (WWTFs) input fresh water, nutrients, and contaminants to the Long Island Sound (LIS). While nutrient loads and concentrations for some pollutants are regulated, there are many emerging contaminants that are not controlled as the full range of toxic effects are still to be determined, and the regulatory framework controlling their usage and allowable inputs into coastal waters has yet to be established. The water and sediment of the LIS are routinely sampled for concentration data of classical persistent organic pollutants, however there are numerous emerging contaminants, with known endocrine disrupting and bioaccumulating properties, that have yet to be detected in this economically important region. It is critically important to investigate the inputs of emerging contaminant throughout the LIS, in order to determine the potential impacts on this estuarine ecosystem. Eight waste water treatment facilities (WWTF) which discharge directly into the LIS were tested for several classes of known endocrine disrupting compounds (EDCs); perfluorinated compounds (PFCs), phthalates esters (PAEs) , phenolic compounds (nonylphenol, octylphenol and bisphenol A) and steroidal estrogens. These EDCs have been detected in many water bodies and sediments, yet partitioning data between these compartments are limited. WWTFs are a known point source of these pollutants; research indicates that biodegradation during secondary treatment can increase concentrations of PFCs in wastewater effluent. The distribution of several of the target compounds between the suspended particulate and dissolved phases in the effluent waters was determined to be a function of the organic carbon content of both phases; organic carbon normalized data indicate that partitioning to dissolve organic matter (DOM) is important as a third phase for several target pollutants. The fate and distribution of target compounds entering the saline estuary from the effluent was further investigated; an important factor in distribution of these target compounds is the scavenging by particulates which increases as a function of ionic strength. The water-sediment distributions of target EDCs in different salinity and sediment quality regions of the LIS are presented. These results are an important first step in the investigation into the role of wastewater organic matter in the transport and distribution of target EDCs in an estuary.

MO 180

Assessment of intersex severity in grey mullets from three Portuguese estuaries - preliminary data

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All over the world, plentiful chemicals reach continuously the environment, and some of them are endocrine disrupters compounds (CDEs) which can cause diverse harmful effects in wild fish (also under low concentration) including intersex condition, namely ovotestis (oocytes in the testis), but can also affect human health.
The presence of intersex condition in ichthyofauna has been reported in numerous countries, including (scarce information) in Portugal, but no data was published based on a large sampling and covering several estuaries, and usually no ranking system for severity assessment is done. For this aim, we have been studying adult grey mullets (Mugil cephalus) caught in the estuaries of the rivers Mondego (2006), Douro (2007) and Ave (2008). Collections took place twice a year, aiming 50 animals per survey, in spring/summer (SS) and autumn/winter (AW).
So far, testis histopathology showed intersex condition (ovotestis) at the following rates (SS vs AW): 12 % vs 8 % in Mondego; 30 % vs 8 % in Douro, and 13 % vs 39 % in Ave. Despite the presence of ovotestis in all estuaries, the density and oocyte development stage in testis varies greatly.
We used the Ovotestis Severity Index (OSI) in this work (proposed by Bateman et al. 2004). OSI data obtain are (SS vs AW): 0,6 and 0,3 in Mondego mullets, 6,1 and 2,8 in Douro mullets, and 12,0 and 5,8 in Ave mullets. The OSI was low in Mondego fish, which agree with the less contaminated estuary studied (our reference estuary). In Douro, the fish present higher OSI, but Ave mullet show the highest value. No seasonal differences were detected in OSI values.
In some cases we observed also considerable differences in histopathology of the gonads (fibrosis, melanomacrophage centers, interstitial inflammation, as well as unspecific and parasitic granulomas). The estuaries presenting higher rate of OSI, correspond to the higher pollution levels, and show also higher rate of gonad lesions. These data are in correspondence with our published chemical data, as both Mondego and Douro have estrogens in the water (with a lesser load in Mondego). This work corroborate that mullet are waterborne exposed to estrogenic compounds and OSI should be used in this kind of studies.
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MO 181

Effects of antiandrogenic compounds on roach (Rutilus rutilus) steroidogenesis : an in-situ study based on environmental occurrence and relevant gene expression analysis in gonads

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Wildlife is exposed to an increasing pollution pressure which can disrupt homeostasis and ultimately fitness of the more sensitive species and may thus lead to biodiversity erosion. For more than a decade, efforts were made by the scientific community, to assess and understand the impact of endocrine disruptors, especially estrogenic compounds, on fish breeding cycle. Feminization and demasculinization of fish were demonstrated in the field and correlated not only to estrogenic contaminants but also to antiandrogenic compounds. Although less characterized, these latter might be of importance. They can interfere with the androgen pathways at the receptor level and/or by modulating transcriptional or enzymatic activities related to steroidogenesis. In this study, Roach was chosen with regard to its large repartition in freshwater systems and to its sensitivity to endocrine disruption. Four different sites of the Seine river catchment basin in the Seine presenting an overall contamination gradient were studied. Sediments and fish bile were sampled in order to determine the occurrence of androgen antagonists in the environment and in the exposed animals using the anti-yeast androgen screen (anti-YAS) assay. Liver and gonad of sexually mature individuals were dissected to carry out transcriptional analysis of key genes involved in steroidogenesis. This includes genes encoding for the steroidogenic acute regulatory protein (StAR) responsible of the import of cholesterol in mitochondria that represents the rate limiting step of steroidogenesis; the mitochondrial CYP 11A1 that converts cholesterol to pregnenolone; the CYP 17A1 (17α-hydroxylase/17,20-lyase) that catalyzes oxidation and cleavage of intermediary steroids; the CYP 19A1, so-called aromatase that converts testosterone in estradiol 17-β. Furthermore, transcriptional level of a CYP 3A isoform catalyzing sexual steroid inactivation was assessed in order to appreciate whether environmental pollutants disrupt the biotransformation balance of endogenous steroids. To our knowledge, this is the first in situ study that underlines in the same time the occurrence of androgen receptor antagonists in sediments and antiandrogenic effects on gonadal mRNA levels.

MO 182

Analysis and occurrence of endocrine disruptors and related compounds in surface waters and sediments in rivers of the Iberian Peninsula

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The Mediterranean basin is one of the most vulnerable regions of the world to the global change due their climatic conditions characterized by summer drought and their characteristic topographical regions. Moreover, the high activity close to the Mediterranean rivers and the high population density in these zones, are the principals arguments to evaluate the water quality of these rivers.
The objective of this work was the determination of endocrine disruptors and related compounds belonging to different groups of chemical substances (10 estrogens, natural and synthetic, in free and conjugated form, 8 alkylphenols, 4 antiseptics, 2 antibacterials, 3 flame retardants, 2 anticorrosives and BPA) in four representative watersheds in Spain: Llobregat, Ebro, Júcar, and Guadalquivir.
In this study, a multiresidue analytical method for the analysis of water samples was applied, using the Thermo Scientific Equan LC-MS system, an automated online preconcentration method. For the analysis of sediment samples a pressurized liquid extraction (PLE) was carried out using a fully automated ASE 200 system (Dionex, Sunnyvale, CA, USA), the solvent extraction was methanol:acetone (1:1) mixture, for clean-up a solid phase extraction (SPE) was performed. A Thermo Scientific TSQ Vantatge triple quadrupole mass spectrometer with an ESI source was used for the MS analysis.
The results show widespread occurrence of target compounds, although the level of concentrations of different compounds detected varied considerably depending on the sampling point. For example, in the case of surface waters the 3 chemical groups with higher contribution in terms of concentrations were alkylphenolic, corrosives and orghanophosphorous flame retardants with levels between ng/L to µg/L. The natural and synthetic estrogens in free and conjugated forms were found in some points in levels lower than 10 ng/L.
In order to estimate the estrogenicity of samples, the EEQ were calculated using relative estrogenic potency (relative to 17 β-estradiol). As it was expected, the results showed that estrogens, especially estradiol, were the largest contributors to the estrogenic potential with values between nd-4.60 ng/L. However the contribution of other compounds such as alkylphenols, BPA and anticorrosives to the total estrogencity was low and ranged between nd-0.09 ng/L.

MO 183

Specific accumulation of polychlorinated biphenyls and brominated flame retardants in human breast milk and scalp hair from the Philippines: levels, distribution and profiles

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Due to the lack of adequate treatment facilities, large amount of municipal wastes are directly dumped at dumping sites in the Philippines without proper management, probably causing several adverse environmental consequences and increased human health risk to local communities. Overall, the data on human exposure to organohalogen compounds in the Philippines is rather scarce and comprehensive studies have not been made. The present study was therefore carried out to determine the concentrations of three group of persistent organohalogens such as polychlorinated biphenyls (PCBs), polybrominated diphenyl ethers (PBDEs) and hexabromocyclododecanes (HBCDs) in human breast milk and scalp hair samples from mothers living in two locations in the Philippines, viz., Payatas, a waste dumpsite, and Malate, a non-dumpsite. In addition, the present study examined relationships between contaminant levels in milk/hair samples. Human breast milk and scalp hair samples (n=30) from primipara and multipara mothers living in two locations in the Philippines were obtained in 2008 and analyzed for three groups of organohalogen compounds (PCBs, PBDEs and HBCDs). PCBs were

the predominantly identified compounds in all the breast milk samples. The highest concentrations of PCBs in breast milk (115 ng/g lipid wt., sum of 12 congeners) were found in a sample from a 28-year old woman, living in the periphery of the dumpsite (Payatas) and nursing for the third time. Levels of PBDEs in human breast milk samples from the Philippines were similar to Europe and other Asian countries. Among PBDEs, BDE-47, -99, -100 and -153 were the major congeners. For HBCDs, -isomer was the predominant followed by- isomer in both locations. PBDE concentrations (including BDE -209) were significantly higher than those of PCBs and HBCDs in all the scalp hair samples. On a congener basis, the levels of PBDEs found in scalp hair were higher than those in Spain (children and adults) and China (e-waste workers). PBDE congeners in scalp hair were dominated by those found in Deca- and Penta-BDE mixtures. To our knowledge, this is the first comprehensive research on HBCDs in human scalp hair from the world. Human hair as a biological measure of exposure to persistent organic pollutants has some advantages over the more commonly used blood, milk and adipose tissue samples.

MO 184

Alkylphenolic substances, steroid estrogens and bisphenol A in water, sediment and fish from Dan-Shui River, Taiwan

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This study investigated the distribution of feminizing chemicals including 4-*tert*-octylphenol (OP), 4-nonylphenol (NP), nonylphenol monoethoxycarboxylate (NP_1EC), nonylphenol monoethoxylate (NP_1EO), nonylphenol diethoxylate (NP_2EO), bisphenol A (BPA), estrone, 17β-estradiol, estriol and 17α-ethinyl estradiol in river water, sediment and fish in the Dan-Shui River, Taipei, Taiwan. Sampling was conducted every one and a half months in nine months. The concentrations in fish organs were also determined to estimate the organ distribution and the bioaccumulation of these chemicals. Water, sediment and fish (*Oreochromis mossambicus* and *Oreochromis niloticus*) were taken from the Dan-Shui River. Water was pretreated with automated solid-phase extraction. Sediment and biota were extracted with matrix solid-phase dispersion. The quantification was done with ultra-high performance liquid chromatography/tandem mass spectrometry and isotope dilution techniques.
Alkylphenolic substances and BPA were detected in all of the water samples. BPA was the most abundant analyte in river water (547 ± 602 ng/L). In the tributary of the Dan-Shui River, the concentrations were the highest near a wastewater treatment plant (WWTP). The average concentration of BPA in the main stream of the Dan-Shui River (1,169 ± 906 ng/L) was four times higher than that in the tributary (313 ± 144 ng/L). The spatial variation of concentrations in water were associate with the emission from point sources. NP was the most abundant analyte in sediment (1,131 ± 839 ng/g w.w.) and in fish muscle (245 ± 167 ng/g w.w.). Only few ng/g w.w. of steroid estrogens were detected. Unlike the feminizing chemicals in water, the higher concentrations in the sediment were detected at the downstream of a WWTP.
Although BPA is easy to degrade, up to hundreds of ng/g w.w. were detected in fish muscle. Concentrations of feminizing chemicals in fish organs were found to be higher than that in muscle. NP was abundant in liver (3,036 ± 3,115 ng/g w.w.), gonad (9,597 ± 10,536 ng/g w.w.) and eggs (6,376 ± 5,142 ng/g w.w.). The bioconcentration factors (BCFs) of NP were also the highest among these chemicals (1.1 L/g in muscle, 15.8 L/g in liver and 45.8 L/g in gonad). There might be bioaccumulation of alkylphenolic substances in liver and gonad. Skewed sex ratio (female:male = 1.7) could relate to high concentrations in the organs.

MO 185

Determining outliers in fathead minnow (Pimephales promelas) plasma vitellogenin concentration and their correlation to other assay endpoints

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Plasma vitellogenin concentration is an important biomarker and is a data endpoint collected in the OECD 229, 230 and OPPTS 890.1350 test guidelines used to screen chemicals for potential endocrine activity in sexually mature male and spawning female fathead minnows (Pimephales promelas). Plasma vitellogenin concentration is also an important endpoint in the OECD 234 test guideline in maturing freshwater fish. Due to the inherent variability observed within a typical population of fish, examining historical control data and determining outliers is imperative. The objective of this presentation is to outline historical control ranges of vitellogenin concentrations in plasma and to provide recommendations for considering a sample result to be an outlier. The outlier samples from female fish are typically characterized by low vitellogenin recoveries while the outlier samples from male fish are typically uncharacteristically high vitellogenin recoveries. Samples that do not fall within the typical ranges are most often extreme outliers, often observed to be orders of magnitude different from the expected ranges found in historical control data. Inclusion of these outliers in statistical analysis can skew means and decrease sensitivity of the analysis causing some empirical or statistically significant differences to either be magnified or masked. Exploration of vitellogenin results and correlation to effects observed in the remaining endpoints (i.e. gonad histopathology, percent gonadosomatic index, percent of viable eggs, fecundity, etc.) is also considered when evaluating possible outliers. This correlation is important in deciding if plasma vitellogenin concentration is a stand-alone endpoint where an outlier can be individually excluded or if an outlier should be removed from other endpoints as well. Based on the historical control data base and the procedure for determining outliers within a vitellogenin dataset, there is no indication that the other endpoints are affected in either female or male fish and therefore would not warrant exclusion from further analysis.

MO 186

Application of ultra performance liquid chromatography-tandem mass spectrometry for the determination of steroid estrogens and non-ionic surfactants in wastewaters

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Separate ultra-performance liquid chromatography methods using a triple quadrupole mass spectrometer was developed and validated for the determination of steroid estrogens and alkylphenol ethoxylates in wastewater matrices. To date, analytical methods established in the literature for 17α-ethinylestradiol have been unable to achieve the respective proposed predicted no effect concentration of 0.1 ng l-1. The estrogen analytical method enables 17α-ethinylestradiol to be determined below the PNEC with a method detection limit of 0.06 ng l-1 which has been validated in real environmental matrices. During the validation process, a trickling filter wastewater treatment works was monitored to demonstrate the methods application. Estrogen removal across the filters demonstrated good removals of natural free estrogens (≥62.0 %) with lower removals of synthetic estrogen 17α-ethinylestradiol (29.2 %) from wastewaters at 10 °C. The methods application illustrates the proposed methods capability to detect estrogens below PNEC values in real samples. Furthermore, a complete process mass balance for 17α-ethinylestradiol is now attainable which has previously posed a challenge due to the low environmental concentrations typically exhibited, but more significantly as a result of the lower sensitivity inherent in previously reported analytical methods. The ultra performance liquid chromatography method developed for alkylphenol polyethoxylates enables these compounds to be determined in the ng l-1 range which is crucial due to the reduced concentrations in crude sewage experienced over recent years.

MO 187

Occurrence and behavior of Dechlorane plus, Polybromodiphenyl ethers and Emerging BFRs in raptor eggs from Doñana National Park (south-western Spain)

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Dechloranes 602 (Dec 602), 603 (Dec 603) and 604 (Dec 604), syn- and anti-Dechlorane Plus (sDP and aDP), are halogenated flame retardants introduced as replacements of Mirex. Presence of these emerging pollutants has been observed in sediments and biological matrices such as fish and eggs, showing their bioaccumulation potential. Recent studies report the effects of syn- and anti-DP as endocrine disruptors. Dec 602, Dec 603, and Dec 604 are supposed to have similar toxicological properties than DP. The knowledge about the environmental occurrence, fate and behavior of dechloranes and related compounds is still limited. Moreover, most of the reported levels are near production facilities (China and USA), where the concentration levels of these contaminants is expected to be higher than in other places of the world.
On the other hand, polybrominated diphenyl ethers (PBDEs) have been widely used as flame retardants for many years and concentration levels have been severally reported. Along with other harmful effects, PBDEs are endocrine and thyroid disruptors. Thus, production and use of commercial PBDE mixtures are banned in Europe. However, alternative non-BDE BFRs such as pentabromoethylbenzene (PBEB), hexabromobenzene (hexaBBz) and decabromodiphenylethane (deBDethane) are being developed and used.
The purpose of this study was to determine the occurrence of Dechloranes, PBDEs and emerging BFRs in different raptor eggs. Eggs of white storks (Ciconia ciconia) and black kites (Milvus migrans) were collected during the breeding season of 2011. Additionally, samples of sediments, mullets (Mugil cephalus), carps (Cyprinus carpio), barbels (Luciobarbus sclateri) and red swamp crawfishs (Procambarus clarkii) were also collected for bioaccumulation and bioconcentration studies. Sample preparation methods were developed and optimized for all the flame retardants included in the study, and for all the selected matrixes. Instrumental determination was carried out by GC-NCI-MS for PBDEs and emerging BFRs, whereas Dechloranes were analyzed by GC-NCI-MS-MS method.
Both PBDEs and dechloranes (DP isomers, Dec 602 and Dec 603) were detected in egg samples, as well as in sediments and biota samples collected along the Doñana National Park. This is the first time that these emerging contaminant levels are reported in food webs from Spain. The study of Fanti ratio showed a decrease in the biota samples, suggesting that syn-DP has more bioaccumulation capacity than the anti-DP.

MO 188

Hexabromocyclododecane (HBCDD) a flame retardant with POP-properties used in polystyrene insulation products

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Hexabromocyclododecane (HBCDD or HBCD) is an emerging chemical used mainly as a flame retardant in polystyrene-based building insulation products.
There are 64 theoretical possible isomers, of which only 16 exist and 3 dominate. Commercial products contain mainly the -isomer (75-89%) and less of the - (10-13%) and -isomers (1-12%).
Of particular concern is the capacity of this lipophilic and persistent organic pollutant to accumulate in organisms and magnify in the food chain, leading to progressively increasing background levels in human tissues - including mothers' milk - and in wildlife, especially of the most stable -isomer. The extent of this accumulation correlates directly with its ever-more prevalent use.
Limited toxicological information is available to assess the long-term implications for health or the environment of the HBCDD contamination but HBCDD is an endocrine

disruptor in animals.
In 2008 The European Chemicals Agency identified HBCDD as 1 of 14 substances of "Very High Concern", and in September 2010 HBCDD was added to REACH's Authorization List. In February 2011 HBCDD was selected to be phased out by EU REACH Regulation before 2015, if authorization is not granted.
In October 2010 and October 2011 POP Review Committee under the Stockholm Convention has assessed the risks from HBCDD, and it was concluded that HBCDD fulfils the criteria of a persistent organic pollutant (POP).
This presentation will provide a succinct up-to date overview of HBCDD's properties, uses, and regulation and discusses the risks associated with its prevalence in buildings, our homes and immediate environment.

MO 189
Statistical models for sex ratio data
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Studies following OECD Fish Sexual Development Test (FSDT) Test Guideline 234 call for 50% male and 50% female fish during the sex labile period to be placed in each replicate tank in the control and test concentrations at the start of the experiment, with the primary goal to determine whether the test substance causes sex reversal. The observed percent male has its maximum variance when the true percent is 50%. Thus, all analyses of sex-ratio must deal with high variability. This is quite different from typical survival analysis, where control survival is close to 100%.
This variability affects both ECx and NOEC analyses. For NOECs, there is reduced power to detect an effect. With regression, there are increased model uncertainty and width of confidence intervals for ECx. One idea to reduce variability is to "normalize"sex-ratio by dividing each replicate response by the control mean response. Normlized responses may still be highly variable, since they are ratios of two random variables. Also, such data are no longer independent, since they all have the same random variable demoninator, thereby violating a basic requirement of regression and hypothesis testing models. Mathematical details show that the correlations among the normalized responses are not trivial and cannot be ignored.
The quality of regression models and resulting ECx estimates based on non-normalized responses were investigated using data from numerous studies done following TG234. Numerous well-accepted regression models for toxicity data were fit to the data, goodness-of-fit was assessed, and confidence intervals for ECx estimates for x=5, 10, 20, and 50 were obtained. Several hypothesis tests were used to obtain NOECs. These methods were compared to one another and to the regression results. Both regression and hypothesis test results s were supplemented by computer simulations that showed the conclusions are true in general.

The results show that for fish sex-ratio data based on phenotypic sex, regression models often fail to provide meaningful estimates of ECx for x≤20 and sometimes for larger values of x. This is true regardless for any practical experimental design for the FSDT. The step-down Jonckheere-Terpstra test usually provides meaningful NOEC values that are useful for risk assessment. When genetic sex is known, so true sexual reversal can be measured, the situation is quite different and regression models are very useful.

MO 190
Progress of assessment under the Japanese program on endocrine disruption: EXTEND2010
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Ministry of the Environment, Japan implemented their third research program on endocrine disruption titled "EXTEND2010"(EXTEND: Extended Tasks on Endocrine Disruption) in July 2010. Target of the new five-year program is to accelerate hazard assessment on endocrine disruption of chemical substances, prioritizing organisms in the environment, and to consequently conduct risk assessment to see whether any regulatory risk management measures should be introduced.
Test protocols of fish, amphibian and invertebrates have been developed through bilateral or multilateral collaborations. *In vitro* assays using receptors of fish, amphibians and invertebrates are also being developed in the ministry's program. Two-tiered framework for assessing endocrine disrupting effects to organisms in the environment is being developed. This framework is designed to effectively identify potential candidates for endocrine disruptors using available information and test results. Reliability evaluation of available information that might be relevant to endocrine disruption is being conducted to select candidate chemicals subject to testing to assess their endocrine disrupting effects to aquatic organisms. The existing knowledge is re-evaluated to identify which *in vitro* assays should be conducted for prioritization to select candidate chemicals for *in vivo* tests.
After the two batches of reliability evaluation twenty-five chemicals were identified as candidates for testing. *In vitro* assays were conducted for eighteen chemicals in FY 2010 and 2011 and estrogenic and anti-estrogenic activities were detected in some of them. The way of prioritized selection of chemicals subject to tier 1 *in vivo* testing is being discussed based on the results.
Progress and updated status of the assessment of chemicals under the EXTEND2010 will be demonstrated.

MO 191
Impact of animal manure separation technologies on steroid hormone distribution - consequences for agricultural practices
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When steroid hormones are emitted into the environment, they may have harmful effects on the reproduction system of aquatic life. Until now, research has primarily focused on human excretion, demonstrating that steroid hormones reach the aquatic environment due to insufficient removal in waste water treatment processes. However more recently, it has been revealed that agricultural practices also may add to the environmental burden of steroid hormones. So far, research activities have mainly focused on steroid estrogens, but also androgens, progestagens and glucocorticoids, expressed in the vertebrate steroidogenesis, may occur at substantial levels in animal manure and should be addressed. In agricultural practices the animal manure can be applied to the soil as raw manure, but also as a solid or liquid manure fraction, since current livestock production facilities utilizes a recently developed technology, which separates raw animal manure into a solid and a liquid fraction. This technology offers an improved handling and refined distribution of the manure nutrients to the farmlands and the possibility to reduce the environmental impact of manure nutrients, especially avoiding the surplus load of phosphorous.
In the present work we investigated the distribution of 9 steroid hormones (pregnenolone, progesterone, dehydroepiandrosterone, androstenedione, testosterone, dihydrotestosterone, estrone, 17α-estradiol and 17β-estradiol) in raw manure and manure separates from 10 to 15 different pig farms in Denmark utilizing 4 different separation technologies. Furthermore, we investigated a possible relationship between the steroid hormone concentration and the different manure fractions and separation technologies. The chemical steroid hormone analysis was done by inverse and integrated clean-up pressurized liquid extraction, and further cleaned by a two step solid-phase extraction before derivatization and finally analyzed by GC-MS/MS.
It was found that the steroid hormones were predominant in the solid manure separate calling for manure management strategies to reduce the content of steroid hormones in separated manure solid fraction. This could potentially be achieved through composting or anaerobic digestion for biogas production of the solid fraction; however, the effects of these technologies on steroid hormones need to be verified.

MO 192
Criteria for endocrine disrupters: report from the Danish centre on Endocrine Disrupters (CEHOS)
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The aim of this session is to give a presentation of the report (both ENV and HH) on criteria carried out by the Danish Centre on Endocrine Disrupters (CEHOS) as a project contracted by the Danish Environmental Protection Agency. CEHOS is an interdisciplinary scientific network without walls and the main purpose of the Centre is to build and gather new knowledge on endocrine disrupters (EDs) with focus on information needed for the preventive work of the regulatory authorities. The aim of the report was to propose scientific criteria for the identification of ED substances of concern for human health and the environment. A number of issues relevant for the development of criteria for EDs were considered such as definition, potency, lead effects, specificity and relevance for humans and the environment.
The proposed criteria divide substances into three categories dependent on the available data: 1. Confirmed ED, 2a. Suspected ED and 2b. Indicated ED. The report describes the scientific evidence needed for fulfilling these criteria based on the OECD Conceptual Framework for endocrine testing and assessment. It considers non-test methods, test methods, epidemiology and field studies and gives examples of available ED data and relevant placement in groups. The overall purpose of the report is to provide scientific background for Danish input to the ongoing EU work within this field.

EP05P - Non-target analysis and identification of toxicologically significant emerging pollutants

MO 193
Innovative biodiagnosis meets chemical structure elucidation - New tools in effect directed analysis to support the identification and monitoring of emerging toxicants on a European scale (EDA-EMERGE)
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[11]European Commission Joint Research Centre, Ispra, Italy
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EDA-EMERGE aims to train a new generation of young scientists in the interdisciplinary techniques required to meet the major challenges in the monitoring, assessment and management of toxic pollution in European river basins considering the enormous complexity of contamination, effects and cause-effect relationships. By integrating innovative mode-of-action based biodiagnostic tools including in vitro tests, transgenic organisms and "omics"techniques with powerful fractionation and cutting edge analytical and computational structure elucidation tools, a new generation of effect directed analysis (EDA) approaches will be developed for the identification of toxicants in European surface and drinking waters. Innovative method development by young researchers at major universities, research centres and private companies will be closely interlinked with a joint European demonstration program and higher tier EDA and extensive training courses. EDA-EMERGE ESRs will learn to organise and run international and interdisciplinary sampling and monitoring campaigns and benefit from the expertise of one of the most experienced private companies in this field. Strong networking between academia, the private sector and leading regulators in the field of river basin management and pollution management ensures the relevance of the research for practice and excellent employment opportunities for EDA-EMERGE ESRs.

MO 194
Overview of available chemical analytical screening methods for identification of pollutants in European waters
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The need for collection and dissemination of information about the currently applied techniques for analytical screening of chemical pollutants in water has been recognized at European level. These techniques are identified as promising tools for the identification of the pollutants of concern at river basin or local level (river basin specific pollutants) under the Water Framework Directive WFD (2000/60/EC)). They should allow a cost effective overview of the pollutants in the aquatic environment, in preparation of dedicated monitoring programmes.
The Italian Institute for Water Research IRSA, the EC Joint Research Centre and the NORMAN Association (Network of reference laboratories and research centres for emerging pollutants www.norman-network.net) for emerging pollutants have launched a survey for identification of currently available and used screening methods for the identification and quantification of chemical contaminants in water. A questionnaire was sent to the delegates of the chemical monitoring group under the Water Framework Directive Common Implementation Strategy (WFD - CIS) and through the NORMAN network. 20 compiled questionnaires were received. The response covered a wide geographical spread, including UK, Ireland, Portugal, Spain, France, Switzerland, Austria, Germany, The Netherlands, Denmark, Czech Republic and the Slovak Republic.
The survey included questions about the scope of currently employed screening techniques, the instrumental approach and the validation scheme as well as method performance information and target compounds or compound classes. The reported methodologies include multiresidue methods with a defined target compound list, suspect screening techniques without reference standards (i.e. methods which are based on a mass spectra library with a large set of compounds or compound groups) and non-target screening approaches which include the identification of unknown compounds. A wide range and number of chemical pollutants can be covered by the use of liquid chromatography and gas chromatography coupled with mass spectrometer detectors. Methods are in most cases developed and validated in-house. Some of the methodologies are currently in use for monitoring programmes related to the implementation of the WFD. The survey shows that a common understanding of definitions and scopes is essential in exchanging information about most efficient approaches for target, suspect and non-target screening.

MO 195
Ionization pitfalls in nontarget screening by LC-high resolution mass spectrometry
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In nontarget screening approaches using high-resolution mass spectrometry, one important step is the determination of the molecular formula from accurate measured mass and isotope pattern. Similarly, suspect screening approaches derive the exact mass to be searched for from the molecular formula of the compounds of interest. In both cases the formation of protonated (positive ion mode) and deprotonated molecules (negative ion mode), is commonly anticipated when using electrospray (ESI) and atmospheric pressure chemical ionization (APCI). However, for a range of different compound classes, (de-)protonated molecules might be a minor species failing to reach selected intensity thresholds or even be completely absent. This results from (i) adduct formation with solvent or trace contaminant ions, (ii) gas-phase chemical reactions with solvents or trace contaminants, or (iii) electrochemically induced redox reactions at the electrospray needle. While available software tools can account for adducts with well-known species (Na^+, NH_4^+ in positive ion mode; formic acid in negative ion mode) more complex substitution or redox reactions can hardly be addressed. We will present several case studies involving aromatic amines, nitroaromatic compounds or highly chlorinated weak gas-phase acids or bases. We will discuss approaches to allow for a correct assignment of their molecular formula in nontarget screening approaches and how the ions which are likely formed can be derived for different compound classes in suspect screening approaches.

MO 196
RISK-IDENT: assessment of previously unknown anthropogenic trace contaminants
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For the purposes of precautionary environmental protection, the project "RISK-IDENT"develops and applies an identification system for so far unknown anthropogenic trace contaminants in the aquatic system. The degradation of selected trace compounds is tested in lab-scale sewage treatment plants. Column and lysimeter studies are used to characterise mobility. Acute and chronic effect tests will contribute to the risk assessment process. Moreover an innovative elimination method as an additional sewage treatment step based on hydroxyl radicals will be proved.
The starting point of the project is the development of a database for relevant aquatic contaminants which allows an attribution to analytical data from the analysis of real water samples. This is done by
- Acquisition of substance data on the basis of REACH dossiers with particular reference to molecule-specific information (exact mass, log Pow, etc.) of these substances and their likely degradation products
- Observation and application of normalised retention time factors reflecting the molecular hydrophobicity as identification criterion and allowing independent interlaboratory HPLC methods
- Application of three different LC-MS and LC-MS/MS techniques using high-accuracy mass spectrometry for detection of contaminants via the exact mass and multiple-reaction-monitoring (MRM) for target- and nontarget-screening strategies with low- and high resolution tandem mass spectrometers.
- Optimisation of an procedure for identifying previously unknown trace compounds through the computer-aided comparison of analytical features with molecule-specific properties of potential water contaminants.
The poster presents the recently launched project "RISK-IDENT"and illustrates first results of the interlaboratory determination of normalised retention time factors and mass spectrometric information on the way to an independent data base applicable for all laboratories working on the water sector.

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MO 197
Detection and fate of Ionophores in the environment
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Anticoccidial agents or coccidiostatics are the only anti-bacterial substances still authorised as feed additives within the European Union[1]. Anticoccidial agents are used for the prevention and treatment of the disease coccidiosis, which is caused by a unicellular intestinal parasite. Coccidiosis is a major serious disease in poultry as well as in many other hosts.

Ionophores are the most heavily applied sup-group of the two sub-groups of anticoccidial agents, because they also have antibacterial properties. After the ban of antibiotic growth promoters ionophores are used extensively worldwide as prophylactic chemotherapeutics and growth promoters in livestock production. As an example, the yearly consumptions of active compounds are more than 10 tonnes in Denmark and for the Republic of Korea more than 800 tonnes[2-3]. In long term, this may cause problems with resistance development in the treatment of coccidiosis.
Several reports have revealed that ionophores are emerging environmental contaminants in agricultural run-off waters, surface waters, sediments, and ground waters, due to their continuously increased and constant application as feed additives in modern livestock production[2,4-5]. Recent investigations have further reported that transformation

products of certain veterinary drugs such as antibacterial agents (i.e. tetracyclines) possess environmental effects on the soil-bacterial community at similar level as their parent compounds[6]. This has previous also been observed for antibacterial agents[7].
The focus of this study is on general analytical methods for detection of ionophores and unknown transformation products in various matrices. The hyphenated method consists of an integrated clean-up with solid phase extraction followed by high-performance liquid chromatography tandem mass spectrometry (SPE-LC-MS-MS).
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MO 198
Prioritization of emerging pollutants on the basis of chemical structure
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The prioritization of hazardous chemicals is a useful procedure for the identification of critical substances and the optimization of experiments. This procedure became of particular relevance within the EU-REACH regulation, which encourages the minimization of animal testing also by the use of alternative in vitro and in silico methods. Among these methods quantitative structure-activity relationships (QSARs) can predict missing data for the unknown activities and properties necessary to prioritize existing or not yet synthesized chemicals. The prioritization of four classes of emerging pollutants (brominated flame retardants, fragrances, perfluorinated compounds and (benzo)triazoles) is one of the topics of the FP7 European project CADASTER (CAse studies on the Development and Application of in-Silico Techniques for Environmental hazard and Risk assessment). The final goal of the project is to exemplify the integration of information, models and strategies for carrying out hazard and risk assessments for large numbers of substances, organized in the four representative chemical classes.
The prioritization applied to CADASTER chemicals was crucial to focus the experimental design on critical substances on the basis of their chemical structure and potential ecotoxicological hazard.
The aim of this poster is to summarize the prioritizations performed within CADASTER project, also by applying "*ad hoc*"QSAR/QSPR models developed so far (WP3) for the four classes of compounds under investigation. Different prioritization procedures were applied to over 1000 chemicals by combining, through different approaches (similarity analysis, multivariate ranking methods, factorial design), the structural information, encoded in theoretical molecular descriptors, and the data (experimental or predicted) available for different toxicological and ecotoxicological endpoints. Chemicals belonging to the ECHA pre-registration list were also studied in the prioritizations. Priority compounds were suggested for focusing the experiments executed by other CADASTER partners (WP2).

MO 199
Studying nitrophenols as abiotic transformation products of phenolic microcontaminants in wastewater
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For many emerging contaminants in wastewater, biological treatment is incomplete. Rather than removal by mineralization, Sewage Treatment Plant (STP) processes lead to the formation of transformation products through the interaction of these compounds with the organisms in the sludge.[1] Recent publications have classified certain transformations as 'biological', i.e. involving direct interaction with living organisms, and others as 'abiotic,' implying they take place due to reactions with chemical species present in the milieu.[2,3]
One form of abiotic transformation previously observed in STPs is the nitration of phenolic contaminants, forming their corresponding nitrophenol derivatives.[2,3] Nitrophenols have toxic properties.[4] We are investigating the nitration of phenols further to understand both the mechanism and its occurrence in STPs. Initially, we postulate that the nitration is due to the known reaction of a phenol with nitrogen dioxide (-NO_2), through a radical mechanism described by Beake et al.[5]
The source of -NO_2 is nitrite.[5] Nitrite exists in equilibrium with its unionized form, HNO_2, which decomposes slowly leading to the formation, via -NO, of -NO_2.
The nitration was first studied in batch experiments with phenol-containing compounds, including morphine. The time scale of the reaction warranted the development of a fast and direct sampling and analysis method for LC-MS/MS. Although the nitration is complete within a few hours, we are able to measure its progress. The evidence suggests that it is dependant on the concentration of nitrite, the pH, and involves radical intermediates.
Early experiments on morphine suggest that the formation of nitro-morphine by this reaction pathway would only occur in high-nitrite, low-pH conditions in the sludge. It remains to be seen if such conditions could arise under regular STP operation. In order to determine if the results from the batch experiments correctly reflect a real STP, we will analyze effluent for the presence of nitrophenols. We have developed methods for this analysis based on solid-phase extraction. The goals are to elucidate the environmental significance of this abiotic transformation and gain evidence to support a proposed mechanism.

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MO 200
Linear solvation energy relationship models applied as classifiers in non-target analysis - a gas chromatographic approach
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The identification of unknown substances in complex environmental mixtures plays an important role in effect-directed analysis (EDA). Our approach for the identification of unknowns is based on the generation of possible structures followed by the progressive exclusion of structures that do not match experimental chromatographic and spectroscopic behaviour sufficiently. Linear Solvation Energy Relationships (LSERs) are applied as classifiers to predict the logarithmic retention factors log *k* in isocratic Gas Chromatographic (GC) measurements from the structures of candidate compounds. To demonstrate retention prediction and the application of the classifier model, twelve compounds with the molecular formula $C_{12}H_{10}O_2$ were selected, while experimental log *k* values were compared to the predicted values and exclusion of potential candidate compounds was performed. Predicted retention factors gained from calculated substance descriptors show poor quality. Prediction was enhanced by using experimental determined descriptors, also achieved by the GC measurements.

MO 201
Quantitative determination of different ether species in surface waters by Solid Phase Extraction and GC/MS
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Numerous ether species are of growing concern to human health as well as the environment. The production and use of ethers has been rising in many industrial sectors together with the exposure of these compounds to humans. There is a common lack of available information on the use, exposure and toxicity of these compounds. In this study method was developed for the extraction and enrichment of six compounds from the ether family: etbe, 1,4-dioxane, monoglyme, diglyme, triglyme and tetraglyme. These compounds are of concern because they easily dissolve in water and do not partition to soils, entering ground water systems and likely contaminating public water systems. They do not breakdown easily and might be difficult to remove from ground water sources.
Glymes are saturated polyethers which have found a widespread application in manufacturing of products such as printing inks, paints, coatings and batteries. They are also commonly used as reaction solvents in the area of pharmaceuticals or specialty chemicals production. Glymes have been found to be toxic to the reproductive and/or developmental systems causing infertility and harm to the unborn child. 1,4-dioxane has been widely used as a stabilizer for chlorinated solvents. It is also utilized in products such as paint strippers, dyes and greases. Based on the available data 1,4-dioxane is possibly carcinogenic to humans. The use of Etbe as an oxygenate gasoline additive in the production of gasoline is modest, but increasing. It has not been proven to pose any toxicity to humans.
In order to determine six ether compounds in the water samples, solid phase extraction procedure reflecting the method developed by the EPA for the determination of 1,4-dioxane in drinking water was utilized. 500 ml of a sample was passed through a charcoal containing cartridge and eluted with 10 ml of dichloromethane. All of the extracts where analyzed using a Gas Chormatography/Mass Spectrometry (GC/MS) in the selected ion monitoring (SIM) mode. To validate the method for all of the compounds a recovery study was performed, as well as a method detection limit was calculated for each ether. The same extraction procedure was used to determine the concentration of analytes of interest in the surface waters in Germany. Samples from six surface water bodies (Rhein, Main, Lippe, Wesel-Datteln Canal, Schwarzbach, Auesee) in twenty four different locations were collected, extracted and analyzed.

MO 202
UPLC/qTOF/MS and in silico screening for transformation products of pharmaceuticals in water/sediment tests
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Pharmaceuticals are widespread pollutants in the aquatic environment. Laboratory studies showed that the microbial community in river sediments is capable of transforming a variety of pharmaceuticals, and in some river systems this process is the dominating attenuation mechanism. In order to discriminate attenuation of pharmaceuticals along a river from dilution, suitable tools are needed. Among others, the determination of characteristic transformation products could be one such tool. The aim of this study was therefore to elucidate the transformation of several pharmaceuticals in river sediment and to evaluate this approach.